

(19) World Intellectual Property Organization  
International Bureau



(43) International Publication Date  
10 May 2007 (10.05.2007)

PCT

(10) International Publication Number  
**WO 2007/053486 A2**

(51) International Patent Classification:  
**G06F 19/00** (2006.01)

(21) International Application Number:  
PCT/US2006/042140

(22) International Filing Date: 30 October 2006 (30.10.2006)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:

60/730,882	28 October 2005 (28.10.2005)	US
60/732,154	2 November 2005 (02.11.2005)	US
60/737,744	18 November 2005 (18.11.2005)	US
60/758,528	13 January 2006 (13.01.2006)	US
60/780,518	9 March 2006 (09.03.2006)	US
60/788,694	4 April 2006 (04.04.2006)	US
60/812,590	12 June 2006 (12.06.2006)	US
60/815,253	21 June 2006 (21.06.2006)	US

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(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

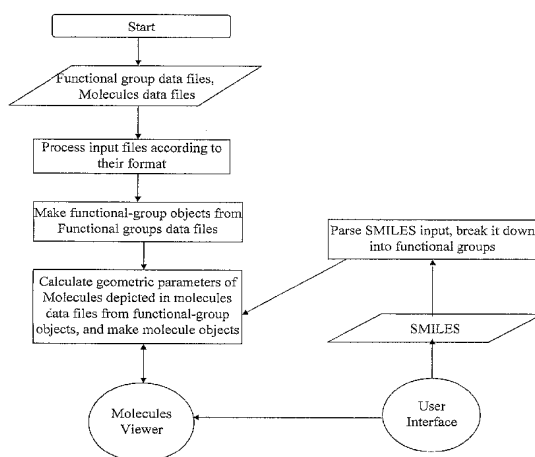
(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

**Published:**

— without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: SYSTEM AND METHOD OF COMPUTING AND RENDERING THE NATURE OF POLYATOMIC MOLECULES AND POLYATOMIC MOLECULAR IONS



(57) Abstract: A method and system of physically solving the charge, mass, and current density functions of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species using Maxwell's equations and computing and rendering the physical nature of the chemical bond using the solutions. The results can be displayed on visual or graphical media. The display can be static or dynamic such that electron motion and specie's vibrational, rotational, and translational motion can be displayed in an embodiment. The displayed information is useful to anticipate reactivity and physical properties. The insight into the nature of the chemical bond of at least one specie can permit the solution and display of those of other species to provide utility to anticipate their reactivity and physical properties.



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## SYSTEM AND METHOD OF COMPUTING AND RENDERING THE NATURE OF POLYATOMIC MOLECULES AND POLYATOMIC MOLECULAR IONS

This application claims priority to U.S. Application Nos.: 60/730,882, filed October 28, 2005; 60/732,154, filed November 2, 2005; 60/737,744, filed November 18, 2005; 60/758,528, filed January 13, 2006; 60/780,518, filed March 9, 2006; 60/788,694, filed April 4, 2006; 60/812,590, filed June 12, 2006; and 60/815,253, June 21, 2006, the complete disclosures of which are incorporated herein by reference.

### Field of the Invention:

This invention relates to a system and method of physically solving the charge, mass, and current density functions of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species, and computing and rendering the nature of these species using the solutions. The results can be displayed on visual or graphical media. The displayed information provides insight into the nature of these species and is useful to anticipate their reactivity, physical properties, and spectral absorption and emission, and permits the solution and display of other species.

Rather than using postulated unverifiable theories that treat atomic particles as if they were not real, physical laws are now applied to atoms and ions. In an attempt to provide some physical insight into atomic problems and starting with the same essential physics as Bohr of the  $e^-$  moving in the Coulombic field of the proton with a true wave equation, as opposed to the diffusion equation of Schrödinger, a classical approach is explored which yields a model that is remarkably accurate and provides insight into physics on the atomic level. The proverbial view deeply seated in the wave-particle duality notion that there is no large-scale physical counterpart to the nature of the electron is shown not to be correct. Physical laws and intuition may be restored when dealing with the wave equation and quantum atomic problems.

Specifically, a theory of classical quantum mechanics (CQM) was derived from first principles as reported previously [reference Nos. 1-8] that successfully applies physical laws to the solution of atomic problems that has its basis in a breakthrough in the understanding of the stability of the bound electron to radiation. Rather than using the postulated Schrödinger boundary condition: " $\Psi \rightarrow 0$  as  $r \rightarrow \infty$ ", which leads to a purely mathematical model of the electron, the constraint is based on experimental observation. Using Maxwell's equations, *the*

*classical wave equation is solved with the constraint that the bound  $n = 1$ -state electron cannot radiate energy.* Although it is well known that an accelerated *point* particle radiates, an *extended distribution* modeled as a superposition of accelerating charges does not have to radiate. A simple invariant physical model arises naturally wherein the predicted results are extremely straightforward and internally consistent requiring minimal math, as in the case of the most famous equations of Newton, Maxwell, Einstein, de Broglie, and Planck on which the model is based. No new physics is needed; only the known physical laws based on direct observation are used.

Applicant's previously filed WO2005/067678 discloses a method and system of physically solving the charge, mass, and current density functions of atoms and atomic ions and computing and rendering the nature of these species using the solutions. The complete disclosure of this published PCT application is incorporated herein by reference.

Applicant's previously filed WO2005/116630 discloses a method and system of physically solving the charge, mass, and current density functions of excited states of atoms and atomic ions and computing and rendering the nature of these species using the solutions. The complete disclosure of this published PCT application is incorporated herein by reference.

Applicant's previously filed U.S. Published Patent Application No. 20050209788A1, relates to a method and system of physically solving the charge, mass, and current density functions of hydrogen-type molecules and molecular ions and computing and rendering the nature of the chemical bond using the solutions. The complete disclosure of this published application is incorporated herein by reference.

### Background of the Invention

The old view that the electron is a zero or one-dimensional point in an all-space probability wave function  $\Psi(x)$  is not taken for granted. The theory of classical quantum mechanics (CQM), derived from first principles, must successfully and consistently apply physical laws on all scales [1-8]. Stability to radiation was ignored by all past atomic models. Historically, the point at which QM broke with classical laws can be traced to the issue of nonradiation of the one electron atom. Bohr just postulated orbits stable to radiation with the further postulate that the bound electron of the hydrogen atom does not obey Maxwell's equations—rather it obeys different physics [1-12]. Later physics was replaced by "pure mathematics" based on the notion of the inexplicable wave-particle duality nature of electrons

which lead to the Schrödinger equation wherein the consequences of radiation predicted by Maxwell's equations were ignored. Ironically, Bohr, Schrödinger, and Dirac used the Coulomb potential, and Dirac used the vector potential of Maxwell's equations. But, all ignored electrodynamics and the corresponding radiative consequences. Dirac originally attempted to solve the bound electron physically with stability with respect to radiation according to Maxwell's equations with the further constraints that it was relativistically invariant and gave rise to electron spin [13]. He and many founders of QM such as Sommerfeld, Bohm, and Weinstein wrongly pursued a planetary model, were unsuccessful, and resorted to the current mathematical-probability-wave model that has many problems [9-16]. Consequently, Feynman for example, attempted to use first principles including Maxwell's equations to discover new physics to replace quantum mechanics [17].

Physical laws may indeed be the root of the observations thought to be "purely quantum mechanical", and it was a mistake to make the assumption that Maxwell's electrodynamic equations must be rejected at the atomic level. Thus, in the present approach, the classical wave equation is solved with the constraint that a bound  $n = 1$ -state electron cannot radiate energy.

Herein, derivations consider the electrodynamic effects of moving charges as well as the Coulomb potential, and the search is for a solution representative of the electron wherein there is acceleration of charge motion without radiation. The mathematical formulation for zero radiation based on Maxwell's equations follows from a derivation by Haus [18]. The function that describes the motion of the electron must not possess spacetime Fourier components that are synchronous with waves traveling at the speed of light. Similarly, nonradiation is demonstrated based on the electron's electromagnetic fields and the Poynting power vector.

It was shown previously [1-8] that CQM gives closed form solutions for the atom including the stability of the  $n = 1$  state and the instability of the excited states, the equation of the photon and electron in excited states, and the equation of the free electron and photon, which predict the wave particle duality behavior of particles and light. The current and charge density functions of the electron may be directly physically interpreted. For example, spin angular momentum results from the motion of negatively charged mass moving systematically, and the equation for angular momentum,  $\mathbf{r} \times \mathbf{p}$ , can be applied directly to the wave function (a current density function) that describes the electron. The magnetic moment of a Bohr magneton, Stern Gerlach experiment, g factor, Lamb shift, resonant line width and

shape, selection rules, correspondence principle, wave particle duality, excited states, reduced mass, rotational energies, and momenta, orbital and spin splitting, spin-orbital coupling, Knight shift, and spin-nuclear coupling, and elastic electron scattering from helium atoms, are derived in closed-form equations based on Maxwell's equations. The calculations agree with experimental observations.

The Schrödinger equation gives a vague and fluid model of the electron. Schrödinger interpreted  $e\Psi^*(x)\Psi(x)$  as the charge-density or the amount of charge between  $x$  and  $x + dx$  ( $\Psi^*$  is the complex conjugate of  $\Psi$ ). Presumably, then, he pictured the electron to be spread over large regions of space. After Schrödinger's interpretation, Max Born, who was working with scattering theory, found that this interpretation led to inconsistencies, and he replaced the Schrödinger interpretation with the probability of finding the electron between  $x$  and  $x + dx$  as

$$\int \Psi(x)\Psi^*(x) dx \quad (1)$$

Born's interpretation is generally accepted. Nonetheless, interpretation of the wave function is a never-ending source of confusion and conflict. Many scientists have solved this problem by conveniently adopting the Schrödinger interpretation for some problems and the Born interpretation for others. This duality allows the electron to be everywhere at one time—yet have no volume. Alternatively, the electron can be viewed as a discrete particle that moves here and there (from  $r = 0$  to  $r = \infty$ ), and  $\Psi\Psi^*$  gives the time average of this motion.

In contrast to the failure of the Bohr theory and the nonphysical, adjustable-parameter approach of quantum mechanics, multielectron atoms [1, 4] and the nature of the chemical bond [1, 5] are given by exact closed-form solutions containing fundamental constants only. Using the nonradiative wave equation solutions that describe the bound electron having conserved momentum and energy, the radii are determined from the force balance of the electric, magnetic, and centrifugal forces that corresponds to the minimum of energy of the system. The ionization energies are then given by the electric and magnetic energies at these radii. The spreadsheets to calculate the energies from exact solutions of one through twenty-electron atoms are given in '06 Mills GUT [1] and are available from the internet [19]. For 400 atoms and ions, as well as hundreds of molecules, the agreement between the predicted and experimental results is remarkable.

The background theory of classical quantum mechanics (CQM) for the physical solutions of atoms and atomic ions is disclosed in R. Mills, *The Grand Unified Theory of*

*Classical Quantum Mechanics*, January 2000 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '00 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, September 2001 Edition, BlackLight Power, Inc., Cranbury, New Jersey, Distributed by Amazon.com (" '01 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, July 2004 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '04 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, January 2005 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '05 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512 (posted at [www.blacklightpower.com](http://www.blacklightpower.com)); R. L. Mills, "The Grand Unified Theory of Classical Quantum Mechanics", June 2006 Edition, Cadmus Professional Communications-Science Press Division, Ephrata, PA, ISBN 0963517171, Library of Congress Control Number 2005936834, (" '06 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512 (posted at <http://www.blacklightpower.com/bookdownload.shtml>); in prior PCT applications PCT/US02/35872; PCT/US02/06945; PCT/US02/06955; PCT/US01/09055; PCT/US01/25954; PCT/US00/20820; PCT/US00/20819; PCT/US00/09055; PCT/US99/17171; PCT/US99/17129; PCT/US 98/22822; PCT/US98/14029; PCT/US96/07949; PCT/US94/02219; PCT/US91/08496; PCT/US90/01998; and PCT/US89/05037 and U.S. Patent No. 6,024,935; the entire disclosures of which are all incorporated herein by reference (hereinafter "Mills Prior Publications").

The following list of references, which are also incorporated herein by reference in their entirety, are referred to in the above sections using [brackets]:

1. R. L. Mills, "The Grand Unified Theory of Classical Quantum Mechanics", June 2006 Edition, Cadmus Professional Communications-Science Press Division, Ephrata, PA, ISBN 0963517171, Library of Congress Control Number 2005936834; posted at <http://www.blacklightpower.com/bookdownload.shtml>.
2. R. L. Mills, "Classical Quantum Mechanics", Physics Essays, Vol. 16, No. 4, December, (2003), pp. 433-498; posted with spreadsheets at [www.blacklightpower.com/techpapers.shtml](http://www.blacklightpower.com/techpapers.shtml).

3. R. Mills, "Physical Solutions of the Nature of the Atom, Photon, and Their Interactions to Form Excited and Predicted Hydrino States", submitted.
4. R. L. Mills, "Exact Classical Quantum Mechanical Solutions for One- Through Twenty-Electron Atoms", in press, posted with spreadsheets at <http://www.blacklightpower.com/techpapers.shtml>.
5. R. L. Mills, "The Nature of the Chemical Bond Revisited and an Alternative Maxwellian Approach", Physics Essays, Vol. 17, (2004), pp. 342-389, posted with spreadsheets at <http://www.blacklightpower.com/techpapers.shtml>.
6. R. L. Mills, "Maxwell's Equations and QED: Which is Fact and Which is Fiction", in press, posted with spreadsheets at <http://www.blacklightpower.com/techpapers.shtml>.
7. R. L. Mills, "Exact Classical Quantum Mechanical Solution for Atomic Helium Which Predicts Conjugate Parameters from a Unique Solution for the First Time", submitted, posted with spreadsheets at <http://www.blacklightpower.com/theory/theory.shtml>.
8. R. Mills, "The Grand Unified Theory of Classical Quantum Mechanics", Int. J. Hydrogen Energy, Vol. 27, No. 5, (2002), pp. 565-590.
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16. A. Einstein, B. Podolsky, N. Rosen, Phys. Rev., Vol. 47, (1935), p. 777.
17. F. Dyson, "Feynman's proof of Maxwell equations", Am. J. Phys., Vol. 58, (1990), pp.

209-211.

18. Haus, H. A., "On the radiation from point charges", American Journal of Physics, 54, (1986), pp. 1126-1129.

19. <http://www.blacklightpower.com/new.shtml>.

#### SUMMARY OF THE INVENTION

The present invention, an exemplary embodiment of which is also referred to as Millsian software, stems from a new fundamental insight into the nature of the atom. Applicant's new theory of Classical Quantum Mechanics (CQM) reveals the nature of atoms and molecules using classical physical laws for the first time. As discussed above, traditional quantum mechanics can solve neither multi-electron atoms nor molecules exactly. By contrast, CQM produces exact, closed-form solutions containing physical constants only for even the most complex atoms and molecules.

The present invention is the first and only molecular modeling program ever built on the CQM framework. All the major functional groups that make up most organic molecules have been solved exactly in closed-form solutions with CQM. By using these functional groups as building blocks, or independent units, a potentially infinite number of organic molecules can be solved. As a result, the present invention can be used to visualize the exact 3D structure and calculate the heat of formation of almost any organic molecule.

For the first time, the significant building-block molecules of chemistry have been successfully solved using classical physical laws in exact closed-form equations having fundamental constants only. The major functional groups have been solved from which molecules of infinite length can be solved almost instantly with a computer program. The predictions are accurate within experimental error for over 375 exemplary molecules.

Applicant's CQM is the theory that physical laws (Maxwell's Equations, Newton's Laws, Special and General Relativity) must hold on all scales. The theory is based on an often overlooked result of Maxwell's Equations, that an extended distribution of charge may, under certain conditions, accelerate without radiating. This "condition of no radiation" is invoked to solve the physical structure of subatomic particles, atoms, and molecules.

In exact closed-form equations with physical constants only, solutions to thousands of known experimental values arise that were beyond the reach of previous outdated theories. These include the electron spin, g-factor, multi-electron atoms, excited states, polyatomic molecules, wave-particle duality and the nature of the photon, the masses and families of



fundamental particles, and the relationships between fundamental laws of the universe that reveal why the universe is accelerating as it expands. CQM is successful to over 85 orders of magnitude, from the level of quarks to the cosmos. Applicant now has over 65 peer-reviewed journal articles and also books discussing the CQM and supporting experimental evidence.

The molecular modeling market was estimated to be a two-billion-dollar per year industry in 2002, with hundreds of millions of government and industry dollars invested in computer algorithms and supercomputer centers. This makes it the largest effort of computational chemistry and physics.

The present invention's advantages over other models includes: Rendering true molecular structures; Providing precisely all characteristics, spatial and temporal charge distributions and energies of every electron in every bond, and of every bonding atom; Facilitating the identification of biologically active sites in drugs; and Facilitating drug design.

An objective of the present invention is to solve the charge (mass) and current-density functions of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species from first principles. In an embodiment, the solution for the polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species is derived from Maxwell's equations invoking the constraint that the bound electron before excitation does not radiate even though it undergoes acceleration.

Another objective of the present invention is to generate a readout, display, or image of the solutions so that the nature of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species be better understood and potentially applied to predict reactivity and physical and optical properties.

Another objective of the present invention is to apply the methods and systems of solving the nature of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species and their rendering to numerical or graphical form to all atoms and atomic ions.

These objectives and other objectives are obtained by a system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising

physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie; and an output device in communication with the processing means for displaying said physical, Maxwellian solutions of charge, mass, and current density functions of said specie.

Also provided is a composition of matter comprising a plurality of atoms, the improvement comprising a novel property or use discovered by calculation of at least one of a bond distance between two of the atoms, a bond angle between three of the atoms, and a bond energy between two of the atoms, orbital intercept distances and angles, charge-density functions of atomic, hybridized, and molecular orbitals, the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.

The presented exact physical solutions for known species of the group of polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any functional group therein, can be applied to other species. These solutions can be used to predict the properties of other species and engineer compositions of matter in a manner which is not possible using past quantum mechanical techniques. The molecular solutions can be used to design synthetic pathways and predict product yields based on equilibrium constants calculated from the heats of formation. Not only can new stable compositions of matter be predicted, but now the structures of combinatorial chemistry reactions can be predicted.

Pharmaceutical applications include the ability to graphically or computationally render the structures of drugs that permit the identification of the biologically active parts of the specie to be identified from the common spatial charge-density functions of a series of active species. Novel drugs can now be designed according to geometrical parameters and bonding interactions with the data of the structure of the active site of the drug.

The system can be used to calculate conformations, folding, and physical properties, and the exact solutions of the charge distributions in any given specie are used to calculate the fields. From the fields, the interactions between groups of the same specie or between groups on different species are calculated wherein the interactions are distance and relative orientation dependent. The fields and interactions can be determined using a finite-element-analysis approach of Maxwell's equations.

Embodiments of the system for performing computing and rendering of the nature of the polyatomic molecules, polyatomic molecular ions, diatomic molecules, molecular radicals, molecular ions, or any portion of these species using the physical solutions may comprise a general purpose computer. Such a general purpose computer may have any number of basic configurations. For example, such a general purpose computer may comprise a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage device, an input means, such as a keyboard or mouse, a display device, and a printer or other output device. A system implementing the present invention can also comprise a special purpose computer or other hardware system and all should be included within its scope.

Although not preferred, any of the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

#### BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 illustrates a block diagram of an exemplary software program; and Figs. 2 and 3 illustrate pictures of an exemplary software program.

### DETAILED DESCRIPTION OF INVENTION

Organic molecules comprising an arbitrary number of atoms can be solved using the similar principles and procedures as those used to solve alkanes of arbitrary length. Alkanes can be considered to be comprised of the functional groups of  $CH_3$ ,  $CH_2$ , and  $C - C$ . These groups with the corresponding geometrical parameters and energies can be added as a linear sum to give the solution of any straight chain alkane as shown in the Continuous-Chain Alkanes section. Similarly, the geometrical parameters and energies of all functional groups such as alkanes, branched alkanes, alkenes, branched alkenes, alkynes, alkyl fluorides, alkyl chlorides, alkyl bromides, alkyl iodides, alkene halides, primary alcohols, secondary alcohols, tertiary alcohols, ethers, primary amines, secondary amines, tertiary amines, aldehydes, ketones, carboxylic acids, carboxylic esters, amides, N-alkyl amides, N,N-dialkyl amides, urea, acid halides, acid anhydrides, nitriles, thiols, sulfides, disulfides, sulfoxides, sulfones, sulfites, sulfates, nitro alkanes, nitrites, nitrates, conjugated polyenes, aromatics, heterocyclic aromatics, substituted aromatics, and others can be solved. The functional-group solutions can be made into a linear superposition and sum, respectively, to give the solution of any organic molecule. The solutions of the functional groups can be conveniently obtained by using generalized forms of the geometrical and energy equations. The equations and sections that are referenced by not contained in this text refer to those sections and equations of the book by R. L. Mills entitled, "The Grand Unified Theory of Classical Quantum Mechanics", June 2006 Edition, Cadmus Professional Communications-Science Press Division, Ephrata, PA, ISBN 0963517171, Library of Congress Control Number 2005936834; posted at <http://www.blacklightpower.com/bookdownload.shtml> which is incorporated in its entirety by reference.

Consider the case wherein at least two atomic orbital hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum, and the sharing of electrons between two or more such orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals. The force generalized constant  $k'$  of a  $H_2$ -type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\epsilon_0} \quad (15.1)$$

where  $C_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of a chemical bond of the molecule or molecular ion which is 0.75 (Eq. (13.59)) in the case of  $H$  bonding to a central atom and 0.5 (Eq. (14.152)) otherwise, and  $C_2$  is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of the chemical bond. From Eqs. (13.58-13.63), the distance from the origin of the MO to each focus  $c'$  is given by:

$$c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}} \quad (15.2)$$

The internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2C_1 C_2}} \quad (15.3)$$

The length of the semiminor axis of the prolate spheroidal MO  $b = c$  is given by

$$b = \sqrt{a^2 - c'^2} \quad (15.4)$$

And, the eccentricity,  $e$ , is

$$e = \frac{c'}{a} \quad (15.5)$$

From Eqs. (11.207-11.212), the potential energy of the two electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.6)$$

The potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \quad (15.7)$$

The kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.8)$$

And, the energy,  $V_m$ , of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.9)$$

The total energy of the  $H_2$ -type prolate spheroidal MO,  $E_T(H_2MO)$ , is given by the sum of the

energy terms:

$$E_T(H_2MO) = V_e + T + V_m + V_p \quad (15.10)$$

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] \end{aligned} \quad (15.11)$$

where  $n_1$  is the number of equivalent bonds of the MO and applies in the case of functional groups. In the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor. It is 1 for a single bond, 4 for an independent double bond as in the case of the  $CO_2$  and  $NO_2$  molecules, and 9 for an independent triplet bond. Then, the kinetic energy term is multiplied by  $c'_{BO}$  which is 1 for a single bond, 2 for a double bond, and 9/2 for a triple bond.  $c_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of an MO which is 0.75 (Eqs. (13.67-13.73)) in the case of  $H$  bonding to an unhybridized central atom and 1 otherwise, and  $c_2$  is the factor that results in an equipotential energy match of the participating the MO and the at least two atomic orbitals of the chemical bond. Specifically, to meet the equipotential condition and energy matching conditions for the union of the  $H_2$ -type-ellipsoidal-MO and the HOs or AOs of the bonding atoms, the factor  $c_2$  of a  $H_2$ -type ellipsoidal MO may given by (i) one, (ii) the ratio of the Coulombic or valence energy of the AO or HO of at least one atom of the bond and 13.605804 eV, the Coulombic energy between the electron and proton of  $H$ , (iii) the ratio of the valence energy of the AO or HO of one atom and the Coulombic energy of another, (iv) the ratio of the valence energies of the AOs or HOs of two atoms, (v) the ratio of two  $c_2$  factors corresponding to any of cases (ii)-(iv), and (vi) the product of two different  $c_2$  factors corresponding to any of the cases (i)-(v). Specific examples of the factor  $c_2$  of a  $H_2$ -type ellipsoidal MO given in previous sections are

0.936127, the ratio of the ionization energy of  $N$  14.53414 eV and 13.605804 eV, the Coulombic energy between the electron and proton of  $H$ ;

0.91771, the ratio of 14.82575 eV,  $-E_{Coulomb}(C, 2sp^3)$ , and 13.605804 eV;

0.87495, the ratio of 15.55033 eV,  $-E_{Coulomb}(C_{ethane}, 2sp^3)$ , and 13.605804 eV;

0.85252, the ratio of 15.95955 eV,  $-E_{Coulomb}(C_{ethylene}, 2sp^3)$ , and 13.605804 eV;

0.85252, the ratio of 15.95955 eV,  $-E_{Coulomb}(C_{benzene}, 2sp^3)$ , and 13.605804 eV, and

0.86359, the ratio of 15.55033 eV,  $-E_{Coulomb}(C_{alkane}, 2sp^3)$ , and 13.605804 eV.

In the generalization of the hybridization of at least two atomic-orbital shells to form a shell of hybrid orbitals, the hybridized shell comprises a linear combination of the electrons of the atomic-orbital shells. The radius of the hybridized shell is calculated from the total Coulombic energy equation by considering that the central field decreases by an integer for each successive electron of the shell and that the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons. The total energy  $E_T(atom, msp^3)$  ( $m$  is the integer of the valence shell) of the AO electrons and the hybridized shell is given by the sum of energies of successive ions of the atom over the  $n$  electrons comprising total electrons of the at least one AO shell.

$$E_T(atom, msp^3) = -\sum_{m=1}^n IP_m \quad (15.12)$$

where  $IP_m$  is the  $m$ th ionization energy (positive) of the atom. The radius  $r_{msp^3}$  of the hybridized shell is given by:

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{-(Z-q)e^2}{8\pi\epsilon_0 E_T(atom, msp^3)} \quad (15.13)$$

Then, the Coulombic energy  $E_{Coulomb}(atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by

$$E_{Coulomb}(atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} \quad (15.14)$$

In the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  at the initial radius  $r$  of the AO electron:

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} = \frac{8\pi\mu_0 \mu_B^2}{r^3} \quad (15.15)$$

Then, the energy  $E(atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by the sum of  $E_{Coulomb}(atom, msp^3)$  and  $E(magnetic)$ :

$$E(\text{atom}, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \quad (15.16)$$

Consider next that the at least two atomic orbitals hybridize as a linear combination of electrons at the same energy in order to achieve a bond at an energy minimum with another atomic orbital or hybridized orbital. As a further generalization of the basis of the stability of the MO, the sharing of electrons between two or more such hybridized orbitals to form a MO permits the participating hybridized orbitals to decrease in energy through a decrease in the radius of one or more of the participating orbitals. In this case, the total energy of the hybridized orbitals is given by the sum of  $E(\text{atom}, msp^3)$  and the next energies of successive ions of the atom over the  $n$  electrons comprising the total electrons of the at least two initial AO shells. Here,  $E(\text{atom}, msp^3)$  is the sum of the first ionization energy of the atom and the hybridization energy. An example of  $E(\text{atom}, msp^3)$  for  $E(C, 2sp^3)$  is given in Eq. (14.503) where the sum of the negative of the first ionization energy of  $C$ ,  $-11.27671 \text{ eV}$ , plus the hybridization energy to form the  $C2sp^3$  shell given by Eq. (14.146) is  $E(C, 2sp^3) = -14.63489 \text{ eV}$ .

Thus, the sharing of electrons between two  $\text{atom } msp^3$  HOs to form an atom-atom-bond MO permits each participating hybridized orbital to decrease in radius and energy. In order to further satisfy the potential, kinetic, and orbital energy relationships, each  $\text{atom } msp^3$  HO donates an excess of 25% per bond of its electron density to the atom-atom-bond MO to form an energy minimum wherein the atom-atom bond comprises one of a single, double, or triple bond. In each case, the radius of the hybridized shell is calculated from the Coulombic energy equation by considering that the central field decreases by an integer for each successive electron of the shell and the total energy of the shell is equal to the total Coulombic energy of the initial AO electrons plus the hybridization energy. The total energy  $E_T(\text{mol. atom}, msp^3)$  ( $m$  is the integer of the valence shell) of the HO electrons is given by the sum of energies of successive ions of the atom over the  $n$  electrons comprising total electrons of the at least one initial AO shell and the hybridization energy:

$$E_T(\text{mol. atom}, msp^3) = E(\text{atom}, msp^3) - \sum_{m=2}^n IP_m \quad (15.17)$$



where  $IP_m$  is the  $m$ th ionization energy (positive) of the atom and the sum of  $-IP_1$  plus the hybridization energy is  $E(atom, msp^3)$ . Thus, the radius  $r_{msp^3}$  of the hybridized shell is given by:

$$r_{msp^3} = \left( \sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25) \right) \frac{-e^2}{8\pi\epsilon_0 E_T(mol.atom, msp^3)} \quad (15.18)$$

where  $s = 1, 2, 3$  for a single, double, and triple bond, respectively. The Coulombic energy  $E_{Coulomb}(mol.atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by

$$E_{Coulomb}(mol.atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} \quad (15.19)$$

In the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  at the initial radius  $r$  of the AO electron given by Eq. (15.15). Then, the energy  $E(mol.atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by the sum of  $E_{Coulomb}(mol.atom, msp^3)$  and  $E(magnetic)$ :

$$E(mol.atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \quad (15.20)$$

$E_T(atom - atom, msp^3)$ , the energy change of each  $atom msp^3$  shell with the formation of the atom-atom-bond MO is given by the difference between  $E(mol.atom, msp^3)$  and  $E(atom, msp^3)$ :

$$E_T(atom - atom, msp^3) = E(mol.atom, msp^3) - E(atom, msp^3) \quad (15.21)$$

As examples from prior sections,  $E_{Coulomb}(mol.atom, msp^3)$  is one of:

$$E_{Coulomb}(C_{ethylene}, 2sp^3), \quad E_{Coulomb}(C_{ethane}, 2sp^3), \quad E_{Coulomb}(C_{acetylene}, 2sp^3), \quad \text{and}$$

$$E_{Coulomb}(C_{alkane}, 2sp^3);$$

$E_{Coulomb}(atom, msp^3)$  is one of  $E_{Coulomb}(C, 2sp^3)$  and  $E_{Coulomb}(Cl, 3sp^3)$ ;

$$E(mol.atom, msp^3) \quad \text{is} \quad \text{one} \quad \text{of} \quad E(C_{ethylene}, 2sp^3), \quad E(C_{ethane}, 2sp^3),$$

$$E(C_{acetylene}, 2sp^3) E(C_{alkane}, 2sp^3);$$

$$E(atom, msp^3) \text{ is one of } E(C, 2sp^3) \text{ and } E(Cl, 3sp^3);$$

$$E_T(atom - atom, msp^3) \text{ is one of } E(C - C, 2sp^3), E(C = C, 2sp^3), \text{ and } E(C \equiv C, 2sp^3);$$

$$atom \ msp^3 \text{ is one of } C2sp^3, Cl3sp^3$$

$$E_T(atom - atom(s_1), msp^3) \text{ is } E_T(C - C, 2sp^3) \text{ and } E_T(atom - atom(s_2), msp^3) \text{ is}$$

$$E_T(C = C, 2sp^3), \text{ and}$$

$$r_{msp^3} \text{ is one of } r_{C2sp^3}, r_{ethane2sp^3}, r_{ethylene2sp^3}, r_{acetylene2sp^3}, r_{alkane2sp^3}, \text{ and } r_{Cl3sp^3}.$$

In the case of the  $C2sp^3$  HO, the initial parameters (Eqs. (14.142-14.146)) are

$$r_{2sp^3} = \sum_{n=2}^5 \frac{(Z-n)e^2}{8\pi\epsilon_0(e148.25751 \text{ eV})} = \frac{10e^2}{8\pi\epsilon_0(e148.25751 \text{ eV})} = 0.91771a_0 \quad (15.22)$$

$$E_{Coulomb}(C, 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} = \frac{-e^2}{8\pi\epsilon_0 0.91771a_0} = -14.82575 \text{ eV} \quad (15.23)$$

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} = \frac{8\pi\mu_0 \mu_B^2}{(0.84317a_0)^3} = 0.19086 \text{ eV} \quad (15.24)$$

$$\begin{aligned} E(C, 2sp^3) &= \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} \\ &= -14.82575 \text{ eV} + 0.19086 \text{ eV} \\ &= -14.63489 \text{ eV} \end{aligned} \quad (15.25)$$

In Eq. (15.18),

$$\sum_{q=Z-n}^{Z-1} (Z-q) = 10 \quad (15.26)$$

Eqs. (14.147) and (15.17) give

$$E_T(mol.atom, msp^3) = E_T(C_{ethane}, 2sp^3) = -151.61569 \text{ eV} \quad (15.27)$$

Using Eqs. (15.18-15.28), the final values of  $r_{C2sp^3}$ ,  $E_{Coulomb}(C2sp^3)$ , and  $E(C2sp^3)$ , and the resulting  $E_T\left(\overset{BO}{C-C}, C2sp^3\right)$  of the MO due to charge donation from the HO to the MO where

$C-C$  refers to the bond order of the carbon-carbon bond for different values of the parameter  $s$  are given in Table 15.1.

Table 15.1. The final values of  $r_{C2sp^3}$ ,  $E_{Coulomb}(C2sp^3)$ , and  $E(C2sp^3)$  and the resulting  $E_T(C-C, C2sp^3)$  of the MO due to charge donation from the HO to the MO where  $C-C$  refers to the bond order of the carbon-carbon bond.

MO Bond Order (BO)	$s$ 1	$s$ 2	$r_{C2sp^3}(a_0)$ Final	$E_{Coulomb}(C2sp^3)$ (eV) Final	$E(C2sp^3)$ (eV) Final	$E_T(C-C, C2sp^3)$ (eV)
I	1	0	0.87495	-15.55033	-15.35946	-0.72457
II	2	0	0.85252	-15.95955	-15.76868	-1.13379
III	3	0	0.83008	-16.39089	-16.20002	-1.56513
IV	4	0	0.80765	-16.84619	-16.65532	-2.02043

In another generalized case of the basis of forming a minimum-energy bond with the constraint that it must meet the energy matching condition for all MOs at all HOs or AOs, the energy  $E(mol.atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell of each bonding atom must be the average of  $E(mol.atom, msp^3)$  for two different values of  $s$ :

$$E(mol.atom, msp^3) = \frac{E(mol.atom(s_1), msp^3) + E(mol.atom(s_2), msp^3)}{2} \quad (15.28)$$

In this case,  $E_T(atom - atom, msp^3)$ , the energy change of each  $atom msp^3$  shell with the formation of each atom-atom-bond MO, is average for two different values of  $s$ :

$$E_T(atom - atom, msp^3) = \frac{E_T(atom - atom(s_1), msp^3) + E_T(atom - atom(s_2), msp^3)}{2} \quad (15.29)$$

Consider an aromatic molecule such as benzene given in the Benzene Molecule section. Each  $C=C$  double bond comprises a linear combination of a factor of 0.75 of four paired electrons (three electrons) from two sets of two  $C2sp^3$  HOs of the participating carbon atoms. Each  $C-H$  bond of  $CH$  having two spin-paired electrons, one from an initially

unpaired electron of the carbon atom and the other from the hydrogen atom, comprises the linear combination of 75%  $H_2$ -type ellipsoidal MO and 25%  $C2sp^3$  HO as given by Eq. (13.439). However,  $E_T(\text{atom} - \text{atom}, msp^3)$  of the  $C-H$ -bond MO is given by  $0.5E_T(C = C, 2sp^3)$  (Eq. (14.247)) corresponding to one half of a double bond that matches the condition for a single-bond order for  $C-H$  that is lowered in energy due to the aromatic character of the bond.

A further general possibility is that a minimum-energy bond is achieved with satisfaction of the potential, kinetic, and orbital energy relationships by the formation of an MO comprising an allowed multiple of a linear combination of  $H_2$ -type ellipsoidal MOs and corresponding HOs or AOs that contribute a corresponding allowed multiple (e.g. 0.5, 0.75, 1) of the bond order given in Table 15.1. For example, the alkane MO given in the Continuous-Chain Alkanes section comprises a linear combination of factors of 0.5 of a single bond and 0.5 of a double bond.

Consider a first MO and its HOs comprising a linear combination of bond orders and a second MO that shares a HO with the first. In addition to the mutual HO, the second MO comprises another AO or HO having a single bond order or a mixed bond order. Then, in order for the two MOs to be energy matched, the bond order of the second MO and its HOs or its HO and AO is a linear combination of the terms corresponding to the bond order of the mutual HO and the bond order of the independent HO or AO. Then, in general,  $E_T(\text{atom} - \text{atom}, msp^3)$ , the energy change of each  $\text{atom } msp^3$  shell with the formation of each atom-atom-bond MO, is a weighted linear sum for different values of  $s$  that matches the energy of the bonded MOs, HOs, and AOs:

$$E_T(\text{atom} - \text{atom}, msp^3) = \sum_{n=1}^N c_{s_n} E_T(\text{atom} - \text{atom}(s_n), msp^3) \quad (15.30)$$

where  $c_{s_n}$  is the multiple of the BO of  $s_n$ . The radius  $r_{msp^3}$  of the  $\text{atom } msp^3$  shell of each bonding atom is given by the Coulombic energy using the initial energy  $E_{Coulomb}(\text{atom}, msp^3)$  and  $E_T(\text{atom} - \text{atom}, msp^3)$ , the energy change of each  $\text{atom } msp^3$  shell with the formation of each atom-atom-bond MO:

$$r_{msp^3} = \frac{-e^2}{8\pi\epsilon_0\alpha_0 (E_{Coulomb}(\text{atom}, msp^3) + E_T(\text{atom} - \text{atom}, msp^3))} \quad (15.31)$$

where  $E_{Coulomb}(C2sp^3) = -14.825751 \text{ eV}$ . The Coulombic energy  $E_{Coulomb}(mol.atom,msp^3)$  of the outer electron of the  $atom\ msp^3$  shell is given by Eq. (15.19). In the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  (Eq. (15.15)) at the initial radius  $r$  of the AO electron. Then, the energy  $E(mol.atom,msp^3)$  of the outer electron of the  $atom\ msp^3$  shell is given by the sum of  $E_{Coulomb}(mol.atom,msp^3)$  and  $E(magnetic)$  (Eq. (15.20)).  $E_T(atom - atom,msp^3)$ , the energy change of each  $atom\ msp^3$  shell with the formation of the atom-atom-bond MO is given by the difference between  $E(mol.atom,msp^3)$  and  $E(atom,msp^3)$  given by Eq. (15.21). Using Eq. (15.23) for  $E_{Coulomb}(C,2sp^3)$  in Eq. (15.31), the single bond order energies given by Eqs. (15.18-15.27) and shown in Table 15.1, and the linear combination energies (Eqs. (15.28-15.30)), the parameters of linear combinations of bond orders and linear combinations of mixed bond orders are given in Table 15.2.

Table 15.2. The final values of  $r_{C2sp^3}$ ,  $E_{Coulomb}(C2sp^3)$ , and  $E(C2sp^3)$  and the resulting  $E_T\left(C - C^{BO}, C2sp^3\right)$  of the MO comprising a linear combination of  $H_2$ -type ellipsoidal MOs and corresponding HOs of single or mixed bond order where  $c_{s_n}$  is the multiple of the bond order parameter  $E_T(atom - atom(s_n),msp^3)$  given in Table 15.1.

MO Bond Order (BO)	$s_1$	$c_{s_1}$	$s_2$	$c_{s_2}$	$s_3$
1/2I	1	0.5	0	0	0
1/2II	2	0.5	0	0	0
I + 1/2II	1	0.5	2	0.25	0
1/2II + (I + II)	2	0.25	1	0.25	2
3/4II	2	0.75	0	0	0
I + II	1	0.5	2	0.5	0
I + III	1	0.5	3	0.5	0
I + IV	1	0.5	4	0.5	0
II + III	2	0.5	3	0.5	0
II + IV	2	0.5	4	0.5	0
III + IV	3	0.5	4	0.5	0
IV + IV	4	0.5	4	0.5	0

MO Bond Order (BO)	$c_{s_3}$	$r_{C2sp^3}(a_0)$ Final	$E_{Coulomb}(C2sp^3)$ (eV) Final	$E(C2sp^3)$ (eV) Final	$E_T\left(C - C, C2sp^3\right)$ (eV)
1/2I	0	0.89582	-15.18804	-14.99717	-0.36228
1/2II	0	0.88392	-15.39265	-15.20178	-0.56689
I + 1/2II	0	0.87941	-15.47149	-15.28062	-0.64573
1/2II + (I + II)	0.25	0.87363	-15.57379	-15.38293	-0.74804
3/4II	0	0.86793	-15.67610	-15.48523	-0.85034
I + II	0	0.86359	-15.75493	-15.56407	-0.92918
I + III	0	0.85193	-15.97060	-15.77974	-1.14485
I + IV	0	0.83995	-16.19826	-16.00739	-1.37250
II + III	0	0.84115	-16.17521	-15.98435	-1.34946
II + IV	0	0.82948	-16.40286	-16.21200	-1.57711
III + IV	0	0.81871	-16.61853	-16.42767	-1.79278
IV + IV	0	0.80765	-16.84619	-16.65532	-2.02043

Consider next the radius of the AO or HO due to the contribution of charge to more than one bond. The energy contribution due to the charge donation at each atom such as carbon superimposes linearly. In general, the radius  $r_{mol2sp^3}$  of the  $C2sp^3$  HO of a carbon atom of a given molecule is calculated using Eq. (14.514) by considering  $\sum E_{T_{mol}}(MO, 2sp^3)$ , the total energy donation to each bond with which it participates in bonding. The general equation for the radius is given by

$$r_{mol2sp^3} = \frac{-e^2}{8\pi\epsilon_0 \left( E_{Coulomb}(C, 2sp^3) + \sum E_{T_{mol}}(MO, 2sp^3) \right)} \quad (15.32)$$

$$= \frac{e^2}{8\pi\epsilon_0 \left( 14.825751 \text{ eV} + \sum |E_{T_{mol}}(MO, 2sp^3)| \right)}$$

The Coulombic energy  $E_{Coulomb}(mol.atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by Eq. (15.19). In the case that during hybridization, at least one of the spin-paired

AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(\text{magnetic})$  (Eq. (15.15)) at the initial radius  $r$  of the AO electron. Then, the energy  $E(\text{mol.atom}, msp^3)$  of the outer electron of the  $\text{atom } msp^3$  shell is given by the sum of  $E_{\text{Coulomb}}(\text{mol.atom}, msp^3)$  and  $E(\text{magnetic})$  (Eq. (15.20)).

For example, the  $C2sp^3$  HO of each methyl group of an alkane contributes  $-0.92918 \text{ eV}$  (Eq. (14.513)) to the corresponding single  $C-C$  bond; thus, the corresponding  $C2sp^3$  HO radius is given by Eq. (14.514). The  $C2sp^3$  HO of each methylene group of  $C_nH_{2n+2}$  contributes  $-0.92918 \text{ eV}$  to each of the two corresponding  $C-C$  bond MOs. Thus, the radius (Eq. (15.32)), the Coulombic energy (Eq. (15.19)), and the energy (Eq. (15.20)) of each alkane methylene group are

$$\begin{aligned} r_{\text{alkane } C_{\text{methylene}} 2sp^3} &= \frac{-e^2}{8\pi\epsilon_0 \left( E_{\text{Coulomb}}(C, 2sp^3) + \sum E_{T_{\text{alkane}}}(\text{methylene } C-C, 2sp^3) \right)} \\ &= \frac{e^2}{8\pi\epsilon_0 (e14.825751 \text{ eV} + e0.92918 \text{ eV} + e0.92918 \text{ eV})} \\ &= 0.81549a_0 \end{aligned} \quad (15.33)$$

$$E_{\text{Coulomb}}(C_{\text{methylene}} 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 (0.81549a_0)} = -16.68412 \text{ eV} \quad (15.34)$$

$$E(C_{\text{methylene}} 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 (0.81549a_0)} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (0.84317a_0)^3} = -16.49325 \text{ eV} \quad (15.35)$$

In the determination of the parameters of functional groups, heteroatoms bonding to  $C2sp^3$  HOs to form MOs are energy matched to the  $C2sp^3$  HOs. Thus, the radius and the energy parameters of a bonding heteroatom are given by the same equations as those for  $C2sp^3$  HOs. Using Eqs. (15.15), (15.19-15.20), (15.24), and (15.32) in a generalized fashion, the final values of the radius of the HO or AO,  $r_{\text{Atom.HO.AO}}$ ,  $E_{\text{Coulomb}}(\text{mol.atom}, msp^3)$ , and  $E(C_{\text{mol}} 2sp^3)$  are calculated using  $\sum E_{T_{\text{group}}}(MO, 2sp^3)$ , the total energy donation to each bond with which an atom participates in bonding corresponding to the values of  $E_T(C^{BO}-C, C2sp^3)$  of the MO due to charge donation from the AO or HO to the MO given in Tables 15.1 and 15.2.



Table 15.3.A. The final values of  $r_{Atom.HO.AO}$ ,  $E_{Coulomb}(mol.atom,msp^3)$ , and  $E(C_{mol}2sp^3)$  calculated using the values of  $E_T\left(C^{BO}-C,C2sp^3\right)$  given in Tables 15.1 and 15.2.

Atom Hybridiz ation Designat ion	$E_r \left( C - C, C2sp^3 \right)$	$E_r \left( C - C, C2sp^3 \right)$	$E_r \left( C - C, C2sp^3 \right)$	$E_r \left( C - C, C2sp^3 \right)$	$E_r \left( C - C, C2sp^3 \right)$	$r_{Atom, HO, AO}$ Final	$E_{Coulomb} (mol\ atom, msp^3)$ (eV) Final	$E(C_{mol} 2sp^3)$ (eV) Final
1	0	0	0	0	0	0.91771	-14.82575	-14.63489
2	-0.36229	0	0	0	0	0.89582	-15.18804	-14.99717
3	-0.46459	0	0	0	0	0.88983	-15.29034	-15.09948
4	-0.56689	0	0	0	0	0.88392	-15.39265	-15.20178
5	-0.72457	0	0	0	0	0.87495	-15.55033	-15.35946
6	-0.85034	0	0	0	0	0.86793	-15.6761	-15.48523
7	-0.92918	0	0	0	0	0.86359	-15.75493	-15.56407
8	-0.54343	-0.54343	0	0	0	0.85503	-15.91261	-15.72175
9	-1.13379	0	0	0	0	0.85252	-15.95955	-15.76868
10	-1.14485	0	0	0	0	0.85193	-15.9706	-15.77974
11	-0.46459	-0.82688	0	0	0	0.84418	-16.11722	-15.92636
12	-1.34946	0	0	0	0	0.84115	-16.17521	-15.98435
13	-1.3725	0	0	0	0	0.83995	-16.19826	-16.00739
14	-0.46459	-0.92918	0	0	0	0.83885	-16.21952	-16.02866
15	-0.72457	-0.72457	0	0	0	0.836	-16.2749	-16.08404
16	-0.5669	-0.92918	0	0	0	0.8336	-16.32183	-16.13097
17	-0.82688	-0.72457	0	0	0	0.83078	-16.37721	-16.18634
18	-1.56513	0	0	0	0	0.83008	-16.39089	-16.20002
19	-0.64574	-0.92918	0	0	0	0.82959	-16.40067	-16.20961
20	-1.57711	0	0	0	0	0.82948	-16.40286	-16.212
21	-0.72457	-0.92918	0	0	0	0.82562	-16.47951	-16.28865
22	-0.85035	-0.85035	0	0	0	0.82327	-16.52645	-16.33559
23	-1.79278	0	0	0	0	0.81871	-16.61853	-16.42767
24	-1.13379	-0.72457	0	0	0	0.81549	-16.68411	-16.49325
25	-0.92918	-0.92918	0	0	0	0.81549	-16.68412	-16.49325
26	-2.02043	0	0	0	0	0.80765	-16.84619	-16.65532

27	-1.13379	-0.92918	0	0	0	0	0.80561	-16.88872	-16.69786
28	-0.85035	-0.85035	-0.46459	0	0	0	0.80076	-16.99104	-16.80018
29	-0.5669	-0.72457	-0.92918	0	0	0	0.78916	-17.04641	-16.85554
30	-1.13379	-1.13379	0	0	0	0	0.79597	-17.09334	-16.90248
31	-1.34946	-0.92918	0	0	0	0	0.79546	-17.1044	-16.91353
32	-0.46459	-0.92918	-0.92918	0	0	0	0.79340	-17.14871	-16.95784
33	-0.64574	-0.85034	-0.85034	0	0	0	0.79232	-17.17217	-16.98131
34	-0.85035	-0.5669	-0.92918	0	0	0	0.79232	-17.17218	-16.98132
35	-0.72457	-0.72457	-0.92918	0	0	0	0.79085	-17.20408	-17.01322
36	-0.82688	-0.72457	-0.92918	0	0	0	0.78617	-17.30638	-17.11552
37	-0.72457	-0.92918	-0.92918	0	0	0	0.78155	-17.40868	-17.21782
38	-0.92918	-0.72457	-0.92918	0	0	0	0.78155	-17.40869	-17.21783
39	-0.54343	-0.54343	-0.5669	-0.92918	0	0	0.78155	-17.40869	-17.21783
40	-0.92918	-0.85034	-0.85034	0	0	0	0.77945	-17.45561	-17.26475
41	-0.82688	-0.92918	-0.92918	0	0	0	0.77699	-17.51099	-17.32013
42	-0.92918	-0.92918	-0.92918	0	0	0	0.77247	-17.6133	-17.42244
43	-0.85035	-0.54343	-0.5669	-0.92918	0	0	0.76801	-17.71561	-17.52475
44	-1.34946	-0.64574	-0.92918	0	0	0	0.76652	-17.75013	-17.55927
45	-0.85034	-0.54343	-0.60631	-0.92918	0	0	0.76631	-17.75502	-17.56415
46	-1.1338	-0.92918	-0.92918	0	0	0	0.7636	-17.81791	-17.62705
47	-0.46459	-0.85035	-0.85035	-0.92918	0	0	0.75924	-17.92022	-17.72936
48	-0.82688	-1.34946	-0.92918	0	0	0	0.75877	-17.93128	-17.74041
49	-1.13379	-1.13379	-1.13379	0	0	0	0.74646	-18.22712	-18.03626
50	-1.79278	-0.92918	-0.92918	0	0	0	0.73637	-18.47690	-18.28604

Table 15.3.B. The final values of  $r_{Atom.HO.AO}$ ,  $E_{Coulomb}(mol.atom,msp^3)$ , and  $E(C_{mol}2sp^3)$  calculated for heterocyclic groups using the values of  $E_T\left(C^{BO}-C,C2sp^3\right)$  given in Tables 15.1 and 15.2.

Atom Hybridization Designation	$E_T \left( C - C, C2sp^3 \right)^{BO}$	$E_T \left( C - C, C2sp^3 \right)^{BO}$	$E_T \left( C - C, C2sp^3 \right)^{BO}$	$E_T \left( C - C, C2sp^3 \right)^{BO}$	$E_T \left( C - C, C2sp^3 \right)^{BO}$	$r_{Atom, HO, AO}$ Final	$E_{Coulomb} (mol, atom, msp^3)$ (eV) Final	$E(C_{mol} 2sp^3)$ (eV) Final
1	0	0	0	0	0	0.91771	-14.82575	-14.63489
2	-0.56690	0	0	0	0	0.88392	-15.39265	-15.20178
3	-0.72457	0	0	0	0	0.87495	-15.55033	-15.35946
4	-0.92918	0	0	0	0	0.86359	-15.75493	-15.56407
5	-0.54343	-0.54343	0	0	0	0.85503	-15.91261	-15.72175
6	-1.13379	0	0	0	0	0.85252	-15.95954	-15.76868
7	-0.60631	-0.60631	0	0	0	0.84833	-16.03838	-15.84752
8	-0.46459	-0.92918	0	0	0	0.83885	-16.21953	-16.02866
9	-0.72457	-0.72457	0	0	0	0.83600	-16.27490	-16.08404
10	-0.92918	-0.60631	0	0	0	0.83159	-16.36125	-16.17038
11	-0.92918	-0.72457	0	0	0	0.82562	-16.47951	-16.28864
12	-0.85035	-0.85035	0	0	0	0.82327	-16.52644	-16.33558
13	-0.92918	-0.92918	0	0	0	0.81549	-16.68411	-16.49325
14	-1.13379	-0.72457	0	0	0	0.81549	-16.68412	-16.49325
15	-1.13379	-0.92918	0	0	0	0.80561	-16.88873	-16.69786
16	-0.85035	-0.85035	-0.46459	0	0	0.80076	-16.99103	-16.80017
17	-0.85034	-0.85034	-0.56690	0	0	0.79597	-17.09334	-16.90247
18	-1.13379	-1.13380	0	0	0	0.79597	-17.09334	-16.90248
19	-0.85035	-0.54343	0.00000	-0.92918	0	0.79340	-17.14871	-16.95785
20	-0.85035	-0.56690	-0.92918	0	0	0.79232	-17.17218	-16.98132
21	-0.54343	-0.54343	-0.56690	-0.92918	0	0.78155	-17.40869	-17.21783
22	-0.85034	-0.28345	-0.54343	-0.92918	0	0.78050	-17.43216	-17.24130
23	-0.92918	-0.92918	-0.92918	0	0	0.77247	-17.61330	-17.42243
24	-0.85034	-0.54343	-0.56690	-0.92918	0	0.76801	-17.71560	-17.52474
25	-0.85034	-0.54343	-0.60631	-0.92918	0	0.76631	-17.75502	-17.56416
26	-1.13379	-0.92918	-0.92918	0	0	0.76360	-17.81791	-17.62704

27	-1.13379	-1.13380	-0.72457	0	0	0.76360	-17.81791	-17.62705
28	-0.46459	-0.85035	-0.85035	-0.92918	0	0.75924	-17.92022	-17.72935
29	-1.13380	-1.13379	-0.92918	0	0	0.75493	-18.02252	-17.83166
30	-1.13379	-1.13379	-1.13379	0	0	0.74646	-18.22713	-18.03627

The energy of the MO is matched to each of the participating outermost atomic or hybridized orbitals of the bonding atoms wherein the energy match includes the energy contribution due to the AO or HO's donation of charge to the MO. The force constant  $k'$  (Eq. (15.1)) is used to determine the ellipsoidal parameter  $c'$  (Eq. (15.2)) of the each  $H_2$ -type-ellipsoidal-MO in terms of the central force of the foci. Then,  $c'$  is substituted into the energy equation (from Eq. (15.11)) which is set equal to  $n_1$  times the total energy of  $H_2$  where  $n_1$  is the number of equivalent bonds of the MO and the energy of  $H_2$ ,  $-31.63536831 \text{ eV}$ , Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO. From the energy equation and the relationship between the axes, the dimensions of the MO are solved. The energy equation has the semimajor axis  $a$  as its only parameter. The solution of the semimajor axis  $a$  then allows for the solution of the other axes of each prolate spheroid and eccentricity of each MO (Eqs. (15.3-15.5)). The parameter solutions then allow for the component and total energies of the MO to be determined.

The total energy,  $E_T(H_2MO)$ , is given by the sum of the energy terms (Eqs. (15.6-15.11)) plus  $E_T(AO/HO)$ :

$$E_T(H_2MO) = V_e + T + V_m + V_p + E_T(AO/HO) \quad (15.36)$$

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] + E_T(AO/HO) \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] + E_T(AO/HO) \end{aligned} \quad (15.37)$$

where  $n_1$  is the number of equivalent bonds of the MO,  $c_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of a chemical bond of the group,  $c_2$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of each chemical bond, and  $E_T(AO/HO)$  is the total energy comprising the difference of the energy  $E(AO/HO)$  of at least one atomic or hybrid orbital to which the MO is energy matched and any energy component  $\Delta E_{H_2MO}(AO/HO)$  due to the AO or HO's charge donation to the MO.

$$E_T(AO/HO) = E(AO/HO) - \Delta E_{H_2MO}(AO/HO) \quad (15.38)$$

As specific examples given in previous sections,  $E_T(AO / HO)$  is one from the group of

$$E_T(AO / HO) = E(O2p \text{ shell}) = -E(\text{ionization}; O) = -13.6181 \text{ eV};$$

$$E_T(AO / HO) = E(N2p \text{ shell}) = -E(\text{ionization}; N) = -14.53414 \text{ eV};$$

$$E_T(AO / HO) = E(C, 2sp^3) = -14.63489 \text{ eV};$$

$$E_T(AO / HO) = E_{Coulomb}(Cl, 3sp^3) = -14.60295 \text{ eV};$$

$$E_T(AO / HO) = E(\text{ionization}; C) + E(\text{ionization}; C^+);$$

$$E_T(AO / HO) = E(C_{ethane}, 2sp^3) = -15.35946 \text{ eV};$$

$$E_T(AO / HO) = +E(C_{ethylene}, 2sp^3) - E(C_{ethylene}, 2sp^3);$$

$$E_T(AO / HO) = E(C, 2sp^3) - 2E_T(C = C, 2sp^3) = -14.63489 \text{ eV} - (-2.26758 \text{ eV});$$

$$E_T(AO / HO) = E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) = 16.20002 \text{ eV};$$

$$E_T(AO / HO) = E(C, 2sp^3) - 2E_T(C \equiv C, 2sp^3) = -14.63489 \text{ eV} - (-3.13026 \text{ eV});$$

$$E_T(AO / HO) = E(C_{benzene}, 2sp^3) - E(C_{benzene}, 2sp^3);$$

$$E_T(AO / HO) = E(C, 2sp^3) - E_T(C = C, 2sp^3) = -14.63489 \text{ eV} - (-1.13379 \text{ eV}), \text{ and}$$

$$E_T(AO / HO) = E(C_{alkane}, 2sp^3) = -15.56407 \text{ eV}.$$

To solve the bond parameters and energies,  $c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}}$  (Eq.

(15.2)) is substituted into  $E_T(H_2MO)$  to give

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] + E_T(AO / HO) \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] + E_T(AO / HO) \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(AO / HO) \end{aligned} \quad (15.39)$$

The total energy is set equal to  $E(\text{basis energies})$  which in the most general case is given by



the sum of a first integer  $n_1$  times the total energy of  $H_2$  minus a second integer  $n_2$  times the total energy of  $H$ , minus a third integer  $n_3$  times the valence energy of  $E(AO)$  (e.g.  $E(N) = -14.53414 \text{ eV}$ ) where the first integer can be 1, 2, 3..., and each of the second and third integers can be 0, 1, 2, 3....

$$E(\text{basis energies}) = n_1(-31.63536831 \text{ eV}) - n_2(-13.605804 \text{ eV}) - n_3 E(AO) \quad (15.40)$$

In the case that the MO bonds two atoms other than hydrogen,  $E(\text{basis energies})$  is  $n_1$  times the total energy of  $H_2$  where  $n_1$  is the number of equivalent bonds of the MO and the energy of  $H_2$ ,  $-31.63536831 \text{ eV}$ , Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO:

$$E(\text{basis energies}) = n_1(-31.63536831 \text{ eV}) \quad (15.41)$$

$E_T(H_2MO)$ , is set equal to  $E(\text{basis energies})$ , and the semimajor axis  $a$  is solved.

Thus, the semimajor axis  $a$  is solved from the equation of the form:

$$-\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(AO / HO) = E(\text{basis energies}) \quad (15.42)$$

The distance from the origin of the  $H_2$ -type-ellipsoidal-MO to each focus  $c'$ , the internuclear distance  $2c'$ , and the length of the semiminor axis of the prolate spheroidal  $H_2$ -type MO  $b = c$  are solved from the semimajor axis  $a$  using Eqs. (15.2-15.4). Then, the component energies are given by Eqs. (15.6-15.9) and (15.39).

The total energy of the MO of the functional group,  $E_T(MO)$ , is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms and  $E_T(\text{atom} - \text{atom}, msp^3.AO)$ , the change in the energy of the AOs or HOs upon forming the bond. From Eqs. (15.39-15.40),  $E_T(MO)$  is

$$E_T(MO) = E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \quad (15.43)$$

During bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy  $\bar{E}_{osc}$  is the sum of the Doppler,  $\bar{E}_D$ , and average vibrational kinetic energies,  $\bar{E}_{Kvib}$ :

$$\bar{E}_{osc} = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_{hv} \sqrt{\frac{2\bar{E}_K}{m_e c^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.44)$$

where  $n_1$  is the number of equivalent bonds of the MO,  $k$  is the spring constant of the equivalent harmonic oscillator, and  $\mu$  is the reduced mass. The angular frequency of the reentrant oscillation in the transition state corresponding to  $\bar{E}_D$  is determined by the force between the central field and the electrons in the transition state. The force and its derivative are given by

$$f(R) = -c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (15.45)$$

and

$$f'(a) = 2c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (15.46)$$

such that the angular frequency of the oscillation in the transition state is given by

$$\omega = \sqrt{\frac{\left[ \frac{-3}{a} f(a) - f'(a) \right]}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}{m_e}} \quad (15.47)$$

where  $R$  is the semimajor axis  $a$  or the semiminor axis  $b$  depending on the eccentricity of the bond that is most representative of the oscillation in the transition state,  $c_{BO}$  is the bond-order factor which is 1 for a single bond and when the MO comprises  $n_1$  equivalent single bonds as in the case of functional groups.  $c_{BO}$  is 4 for an independent double bond as in the case of the  $CO_2$  and  $NO_2$  molecules and 9 for an independent triplet bond.  $C_{1o}$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of the oscillatory transition state of a chemical bond of the group, and  $C_{2o}$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond. Typically,  $C_{1o} = C_1$  and  $C_{2o} = C_2$ . The kinetic energy,  $E_K$ , corresponding to  $\bar{E}_D$  is given by Planck's equation for functional groups:

$$\bar{E}_K = \hbar\omega = \hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3 m_e}} \quad (15.48)$$

The Doppler energy of the electrons of the reentrant orbit is

$$\bar{E}_D \cong E_{hv} \sqrt{\frac{2\bar{E}_K}{m_e c^2}} = E_{hv} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} \quad (15.49)$$

$\bar{E}_{osc}$  given by the sum of  $\bar{E}_D$  and  $\bar{E}_{Kvib}$  is

$$\bar{E}_{osc} (group) = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_{hv} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} + E_{vib} \right) \quad (15.50)$$

$E_{hv}$  of a group having  $n_1$  bonds is given by  $E_T (MO) / n_1$  such that

$$\bar{E}_{osc} = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_T (MO) / n_1 \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.51)$$

$E_{T+osc} (Group)$  is given by the sum of  $E_T (MO)$  (Eq. (15.42)) and  $\bar{E}_{osc}$  (Eq. (15.51)):

$$\begin{aligned} E_{T+osc} (Group) &= E_T (MO) + \bar{E}_{osc} \\ &= \left( \left[ -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] \right. \\ &\quad \left. + E_T (AO / HO) + E_T (atom - atom, msp^3 . AO) \right) \\ &\quad \left( 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \\ &= \left( E(basis \text{ energies}) + E_T (atom - atom, msp^3 . AO) \right) \left( 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \end{aligned}$$

(15.52)

The total energy of the functional group  $E_T(\text{group})$  is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms,  $E(\text{basis energies})$ , the change in the energy of the AOs or HOs upon forming the bond ( $E_T(\text{atom} - \text{atom}, msp^3.AO)$ ), the energy of oscillation in the transition state, and the change in magnetic energy with bond formation,  $E_{mag}$ . From Eq. (15.52), the total energy of the group  $E_T(\text{Group})$  is

$$E_T(\text{Group}) = \left( E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \right) \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{Kvib} + E_{mag} \quad (15.53)$$

The change in magnetic energy  $E_{mag}$  which arises due to the formation of unpaired electrons in the corresponding fragments relative to the bonded group is given by

$$E_{mag} = c_3 \frac{2\pi\mu_o e^2 \hbar^2}{m_e^2 r^3} = c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} \quad (15.54)$$

where  $r^3$  is the radius of the atom that reacts to form the bond and  $c_3$  is the number of electron pairs.

$$E_T(\text{Group}) = \left( E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \right) \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} \quad (15.55)$$

The total bond energy of the group  $E_D(\text{Group})$  is the negative difference of the total energy of the group (Eq. (15.55)) and the total energy of the starting species given by the sum of  $c_4 E_{initial}(c_4 AO / HO)$  and  $c_5 E_{initial}(c_5 AO / HO)$ :

$$E_D(\text{Group}) = - \left[ \left( E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3, AO) \right) \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] \right. \\ \left. + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r_n^3} - \left( c_4 E_{initial}(AO / HO) + c_5 E_{initial}(c_5 AO / HO) \right) \right] \quad (15.56)$$

In the case of organic molecules, the atoms of the functional groups are energy matched to the  $C2sp^3$  HO such that

$$E(AO / HO) = -14.63489 \text{ eV} \quad (15.57)$$

For examples of  $E_{mag}$  from previous sections:

$$E_{mag}(C2sp^3) = c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o \mu_B^2}{(0.91771a_0)^3} = c_3 0.14803 \text{ eV} \quad (15.58)$$

$$E_{mag}(O2p) = c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o \mu_B^2}{a_0^3} = c_3 0.11441 \text{ eV} \quad (15.59)$$

$$E_{mag}(N2p) = c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o \mu_B^2}{(0.93084a_0)^3} = c_3 0.14185 \text{ eV} \quad (15.60)$$

In the general case of the solution of an organic functional group, the geometric bond parameters are solved from the semimajor axis and the relationships between the parameters by first using Eq. (15.42) to arrive at  $a$ . Then, the remaining parameters are determined using Eqs. (15.1-15.5). Next, the energies are given by Eqs. (15.52-15.59). To meet the equipotential condition for the union of the  $H_2$ -type-ellipsoidal-MO and the HO or AO of the atom of a functional group, the factor  $c_2$  of a  $H_2$ -type ellipsoidal MO in principal Eqs. (15.42) and (15.52) may given by

(i) one:

$$c_2 = 1 \quad (15.61)$$

(ii) the ratio that is less than one of  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), and the magnitude of the

Coulombic energy of the participating AO or HO of the atom,  $E_{Coulomb}(MO.atom,msp^3)$  given by Eqs. (15.19) and (15.31-15.32). For  $|E_{Coulomb}(MO.atom,msp^3)| > 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}} = \frac{13.605804 \text{ eV}}{|E_{Coulomb}(MO.atom,msp^3)|} \quad (15.62)$$

For  $|E_{Coulomb}(MO.atom,msp^3)| < 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}}{\frac{e^2}{8\pi\epsilon_0 a_0}} = \frac{|E_{Coulomb}(MO.atom,msp^3)|}{13.605804 \text{ eV}} \quad (15.63)$$

(iii) the ratio that is less than one of  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), and the magnitude of the valence energy,  $E(valence)$ , of the participating AO or HO of the atom where  $E(valence)$  is the ionization energy or  $E(MO.atom,msp^3)$  given by Eqs. (15.20) and (15.31-15.32). For  $|E(valence)| > 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}} = \frac{13.605804 \text{ eV}}{|E(valence)|} \quad (15.64)$$

For  $|E(valence)| < 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}}{\frac{e^2}{8\pi\epsilon_0 a_0}} = \frac{|E(valence)|}{13.605804 \text{ eV}} \quad (15.65)$$

(iv) the ratio that is less than one of the magnitude of the Coulombic energy of the participating AO or HO of a first atom,  $E_{Coulomb}(MO.atom,msp^3)$  given by Eqs. (15.19) and (15.31-15.32), and the magnitude of the valence energy,  $E(valence)$ , of the participating AO or HO of a second atom to which the first is energy matched where  $E(valence)$  is the

ionization energy or  $E(MO.atom,msp^3)$  given by Eqs. (15.20) and (15.31-15.32). For

$|E_{Coulomb}(MO.atom,msp^3)| > E(valence)$ :

$$c_2 = \frac{|E(valence)|}{|E_{Coulomb}(MO.atom,msp^3)|} \quad (15.66)$$

For  $|E_{Coulomb}(MO.atom,msp^3)| < E(valence)$ :

$$c_2 = \frac{|E_{Coulomb}(MO.atom,msp^3)|}{|E(valence)|} \quad (15.67)$$

(v) the ratio that is less than one of the magnitude of the valence-level energies,  $E_n(valence)$ , of the AO or HO of the  $n$ th participating atom of two that are energy matched where  $E(valence)$  is the ionization energy or  $E(MO.atom,msp^3)$  given by Eqs. (15.20) and (15.31-15.32):

$$c_2 = \frac{E_1(valence)}{E_2(valence)} \quad (15.68)$$

(vi) the factor that is the ratio of the hybridization factor  $c_2(1)$  of the valence AO or HO of a first atom and the hybridization factor  $c_2(2)$  of the valence AO or HO of a second atom to which the first is energy matched where  $c_2(n)$  is given by Eqs. (15.62-15.68); alternatively  $c_2$  is the hybridization factor  $c_2(1)$  of the valence AOs or HOs a first pair of atoms and the hybridization factor  $c_2(2)$  of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = \frac{c_2(1)}{c_2(2)} \quad (15.69)$$

(vii) the factor that is the product of the hybridization factor  $c_2(1)$  of the valence AO or HO of a first atom and the hybridization factor  $c_2(2)$  of the valence AO or HO of a second atom to which the first is energy matched where  $c_2(n)$  is given by Eqs. (15.62-15.69);

alternatively  $c_2$  is the hybridization factor  $c_2(1)$  of the valence AOs or HOs a first pair of atoms and the hybridization factor  $c_2(2)$  of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = c_2(1)c_2(2) \quad (15.70)$$

The hybridization factor  $c_2$  corresponds to the force constant  $k$  (Eqs. (11.65) and (13.58)). In the case that the valence or Coulombic energy of the AO or HO is less than 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), then  $C_2$  corresponding to  $k'$  (Eq. (15.1)) is given by Eqs. (15.62-15.70).

Specific examples of the factors  $c_2$  and  $C_2$  of a  $H_2$ -type ellipsoidal MO of Eq. (15.51) given in following sections are

$$c_2(C2sp^3 HO \text{ to } F) = \frac{E(C, 2sp^3)}{E(F)} c_2(C2sp^3 HO) = \frac{-14.63489 \text{ eV}}{-17.42282 \text{ eV}} (0.91771) = 0.77087;$$

$$C_2(C2sp^3 HO \text{ to } Cl) = \frac{E(Cl)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-12.96764 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.81317;$$

$$C_2(C2sp^3 HO \text{ to } Br) = \frac{E(Br)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-11.81381 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.74081;$$

$$C_2(C2sp^3 HO \text{ to } I) = \frac{E(I)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-10.45126 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.65537;$$

$$c_2(C2sp^3 HO \text{ to } O) = \frac{E(O)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-13.61806 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.85395;$$

$$c_2(H \text{ to } 1^\circ N) = \frac{E(N)}{E(C, 2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.35946 \text{ eV}} = 0.94627;$$

$$c_2(C2sp^3 HO \text{ to } N) = \frac{E(N)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-14.53414 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.91140;$$

$$c_2(H \text{ to } 2^\circ N) = \frac{E(N)}{E(C, 2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.56407 \text{ eV}} = 0.93383;$$

$$C_2(S3p \text{ to } H) = \frac{E(S, 3p)}{E(H)} = \frac{-10.36001 \text{ eV}}{-13.60580 \text{ eV}} = 0.76144;$$

$$C_2(C2sp^3 HO \text{ to } S) = \frac{E(S)}{E(C, 2sp^3)} c_2(C2sp^3 HO) = \frac{-10.36001 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.64965;$$



$$\begin{aligned}
 c_2(O \text{ to } S3sp^3 \text{ to } C2sp^3 HO) &= \frac{E(O)}{E(S)} c_2(C2sp^3 HO) \\
 &= \frac{-13.61806 \text{ eV}}{-10.36001 \text{ eV}} (0.91771); \\
 &= 1.20632
 \end{aligned}$$

$$c_2(S3sp^3) = \frac{E_{Coulomb}(S3sp^3)}{E(H)} = \frac{-11.57099 \text{ eV}}{-13.60580 \text{ eV}} = 0.85045;$$

$$C_2(C2sp^3 HO \text{ to } S3sp^3) = \frac{E(S3sp^3)}{E(C, 2sp^3)} c_2(S3sp^3) = \frac{-11.52126 \text{ eV}}{-14.63489 \text{ eV}} (0.85045) = 0.66951;$$

$$\begin{aligned}
 C_2(S3sp^3 \text{ to } O \text{ to } C2sp^3 HO) &= \frac{E(S, 3sp^3)}{E(O, 2p)} c_2(C2sp^3 HO) \\
 &= \frac{-11.52126 \text{ eV}}{-13.61806 \text{ eV}} (0.91771); \\
 &= 0.77641
 \end{aligned}$$

$$\begin{aligned}
 c_2(O \text{ to } N2p \text{ to } C2sp^3 HO) &= \frac{E(O)}{E(N)} c_2(C2sp^3 HO) \\
 &= \frac{-13.61806 \text{ eV}}{-14.53414 \text{ eV}} (0.91771); \\
 &= 0.85987
 \end{aligned}$$

$$c_2(N2p \text{ to } O2p) = \frac{c_2(C2sp^3 HO \text{ to } N)}{c_2(C2sp^3 HO \text{ to } O)} = \frac{0.91140}{0.85395} = 1.06727;$$

$$C_2(\text{benzene}C2sp^3 HO) = c_2(\text{benzene}C2sp^3 HO) = \frac{13.605804 \text{ eV}}{15.95955 \text{ eV}} = 0.85252;$$

$$\begin{aligned}
 c_2(\text{aryl}C2sp^3 HO \text{ to } O) &= \frac{E(O)}{E(C, 2sp^3)} c_2(\text{aryl}C2sp^3 HO) \\
 &= \frac{-13.61806 \text{ eV}}{-14.63489 \text{ eV}} (0.85252) \quad ; \\
 &= 0.79329
 \end{aligned}$$

$$c_2(H \text{ to aniline } N) = \frac{E(N)}{E(C, 2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.76868 \text{ eV}} = 0.92171;$$

$$\begin{aligned}
 c_2(\text{aryl}C2sp^3 HO \text{ to } N) &= \frac{E(N)}{E(C, 2sp^3)} c_2(\text{aryl}C2sp^3 HO) \\
 &= \frac{-14.53414 \text{ eV}}{-14.63489 \text{ eV}} (0.85252) \quad , \\
 &= 0.84665
 \end{aligned}$$

and

$$C_2(S3p \text{ to aryl-type } C2sp^3HO) = \frac{E(S, 3p)}{E(C, 2sp^3)} = \frac{-10.36001 \text{ eV}}{-15.76868 \text{ eV}} = 0.65700.$$

## MO INTERCEPT ANGLES AND DISTANCES

Consider the general case of Eqs. (13.84-13.95) wherein the nucleus of a  $B$  atom and the nucleus of a  $A$  atom comprise the foci of each  $H_2$ -type ellipsoidal MO of an  $A-B$  bond. The parameters of the point of intersection of each  $H_2$ -type ellipsoidal MO and the  $A$ -atom AO are determined from the polar equation of the ellipse:

$$r = r_0 \frac{1+e}{1+e \cos \theta'} \quad (15.71)$$

The radius of the  $A$  shell is  $r_A$ , and the polar radial coordinate of the ellipse and the radius of the  $A$  shell are equal at the point of intersection such that

$$r_A = (a - c') \frac{1 + \frac{c'}{a}}{1 + \frac{c'}{a} \cos \theta'} \quad (15.72)$$

The polar angle  $\theta'$  at the intersection point is given by

$$\theta' = \cos^{-1} \left( \frac{a}{c'} \left( (a - c') \frac{1 + \frac{c'}{a}}{a_0} - 1 \right) \right) \quad (15.73)$$

Then, the angle  $\theta_{AAO}$  the radial vector of the  $A$  AO makes with the internuclear axis is

$$\theta_{AAO} = 180^\circ - \theta' \quad (15.74)$$

The distance from the point of intersection of the orbitals to the internuclear axis must be the same for both component orbitals such that the angle  $\omega t = \theta_{H_2MO}$  between the internuclear axis and the point of intersection of each  $H_2$ -type ellipsoidal MO with the  $A$  radial vector obeys the following relationship:

$$r_A \sin \theta_{AAO} = b \sin \theta_{H_2MO} \quad (15.75)$$

such that

$$\theta_{H_2MO} = \sin^{-1} \frac{r_A \sin \theta_{AAO}}{b} \quad (15.76)$$

The distance  $d_{H_2MO}$  along the internuclear axis from the origin of  $H_2$ -type ellipsoidal MO to the point of intersection of the orbitals is given by

$$d_{H_2MO} = a \cos \theta_{H_2MO} \quad (15.77)$$

The distance  $d_{AAO}$  along the internuclear axis from the origin of the  $A$  atom to the point of intersection of the orbitals is given by

$$d_{AAO} = c' - d_{H_2MO} \quad (15.78)$$

### BOND ANGLES

Further consider an  $ACB$  MO comprising a linear combination of  $C-A$ -bond and  $C-B$ -bond MOs where  $C$  is the general central atom. A bond is also possible between the  $A$  and  $B$  atoms of the  $C-A$  and  $C-B$  bonds. Such  $A-B$  bonding would decrease the  $C-A$  and  $C-B$  bond strengths since electron density would be shifted from the latter bonds to the former bond. Thus, the  $\angle ACB$  bond angle is determined by the condition that the total energy of the  $H_2$ -type ellipsoidal MO between the terminal  $A$  and  $B$  atoms is zero. The force constant  $k'$  of a  $H_2$ -type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\epsilon_0} \quad (15.79)$$

where  $C_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of a chemical bond of the molecule which is 0.75 (Eq. (13.59)) for a terminal  $A-H$  ( $A$  is  $H$  or other atom) and 1 otherwise and  $C_2$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the chemical bond and is equal to the corresponding factor of Eqs. (15.42) and (15.52). The distance from the origin of the MO to each focus  $c'$  of the  $A-B$  ellipsoidal MO is given by:

$$c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}} \quad (15.80)$$

The internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2C_1 C_2}} \quad (15.81)$$

The length of the semiminor axis of the prolate spheroidal  $A-B$  MO  $b=c$  is given by Eq. (15.4).

The component energies and the total energy,  $E_T(H_2MO)$ , of the  $A-B$  bond are given by the energy equations (Eqs. (11.207-11.212), (11.213-11.217), and (11.239)) of  $H_2$  except that the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor which is 1 for a single bond and when the MO comprises  $n_1$  equivalent single bonds as in the case of functional groups.  $c_{BO}$  is 4 for an independent double bond as in the case of the  $CO_2$  and  $NO_2$  molecules. The kinetic energy term is multiplied by  $c'_{BO}$  which is 1 for a single bond, 2 for a double bond, and 9/2 for a triple bond. The electron energy terms are multiplied by  $c_1$ , the fraction of the  $H_2$ -type ellipsoidal MO basis function of a terminal chemical bond which is 0.75 (Eq. (13.233)) for a terminal  $A-H$  ( $A$  is  $H$  or other atom) and 1 otherwise. The electron energy terms are further multiplied by  $c'_2$ , the hybridization or energy-matching factor that results in an equipotential energy match of the participating at least two atomic orbitals of each terminal bond. Furthermore, when  $A-B$  comprises atoms other than  $H$ ,  $E_T(atom - atom, msp^3.AO)$ , the energy component due to the AO or HO's charge donation to the terminal MO, is added to the other energy terms to give  $E_T(H_2MO)$ :

$$E_T(H_2MO) = \frac{-e^2}{8\pi\epsilon_0 c'} \left[ c_1 c'_2 \left( 2c_{BO} - c'_{BO} \frac{a_0}{a} \right) \ln \frac{a+c'}{a-c'} - 1 \right] + E_T(atom - atom, msp^3.AO) \quad (15.82)$$

The radiation reaction force in the case of the vibration of  $A-B$  in the transition state corresponds to the Doppler energy,  $E_D$ , given by Eq. (11.181) that is dependent on the motion of the electrons and the nuclei. The total energy that includes the radiation reaction of the  $A-B$  MO is given by the sum of  $E_T(H_2MO)$  (Eq. (15.82)) and  $\bar{E}_{osc}$  given Eqs. (11.213-11.220), (11.231-11.236), and (11.239-11.240). Thus, the total energy  $E_T(A-B)$  of the  $A-B$  MO including the Doppler term is

$$E_T(A-B) = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2' \left( 2c_{BO} - c_{BO}' \frac{a_0}{a} \right) \ln \frac{a+c'}{a-c'} - 1 \right] + E_T(\text{atom-atom, msp}^3 \text{ AO}) \right) \right] \left[ 1 + \sqrt{\frac{c_{BO} \frac{C_{10} C_{20} e^2}{4\pi\epsilon_0 a^3}}{m_e c^2}} + \frac{1}{2} \sqrt{\frac{c_{BO} \frac{c_1 c_2' e^2}{8\pi\epsilon_0 a^3} - \frac{c_{BO} e^2}{8\pi\epsilon_0 (a+c')^3}}{\mu}} \right] \quad (15.83)$$

where  $C_{10}$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of the oscillatory transition state of the  $A-B$  bond which is 0.75 (Eq. (13.233)) in the case of  $H$  bonding to a central atom and 1 otherwise,  $C_{20}$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond, and

$\mu = \frac{m_1 m_2}{m_1 + m_2}$  is the reduced mass of the nuclei given by Eq. (11.154). To match the boundary

condition that the total energy of the  $A-B$  ellipsoidal MO is zero,  $E_T(A-B)$  given by Eq. (15.83) is set equal to zero. Substitution of Eq. (15.81) into Eq. (15.83) gives

$$0 = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2' \left( 2c_{BO} - c_{BO}' \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(\text{atom-atom, msp}^3 \text{ AO}) \right) \right] \left[ 1 + \sqrt{\frac{c_{BO} \frac{C_{10} C_{20} e^2}{4\pi\epsilon_0 a^3}}{m_e c^2}} + \frac{1}{2} \sqrt{\frac{c_{BO} \frac{c_1 c_2' e^2}{8\pi\epsilon_0 a^3} - \frac{c_{BO} e^2}{8\pi\epsilon_0 \left( a + \sqrt{\frac{aa_0}{2C_1 C_2}} \right)^3}}{\mu}} \right] \quad (15.84)$$

The vibrational energy-term of Eq. (15.84) is determined by the forces between the central field and the electrons and those between the nuclei (Eqs. (11.141-11.145)). The electron-central-field force and its derivative are given by

$$f(a) = -c_{BO} \frac{c_1 c_2' e^2}{4\pi\epsilon_0 a^3} \quad (15.85)$$

and

$$f'(a) = 2c_{BO} \frac{c_1 c_2' e^2}{4\pi\epsilon_0 a^3} \quad (15.86)$$

The nuclear repulsion force and its derivative are given by

$$f(a+c') = \frac{e^2}{8\pi\epsilon_0 (a+c')^2} \quad (15.87)$$

and

$$f'(a+c') = -\frac{e^2}{4\pi\epsilon_0 (a+c')^3} \quad (15.88)$$

such that the angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{\left[ \frac{-3}{a} f(a) - f'(a) \right]}{\mu}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO} \frac{c_1 c_2' e^2}{4\pi\epsilon_0 a^3} - \frac{e^2}{8\pi\epsilon_0 (a+c')^2}}{\mu}} \quad (15.89)$$

Since both terms of  $\bar{E}_{osc} = \bar{E}_D + \bar{E}_{Kvib}$  are small due to the large values of  $a$  and  $c'$ , to very good approximation, a convenient form of Eq. (15.84) which is evaluated to determine the bond angles of functional groups is given by

$$0 = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2' \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T (atom - atom, msp^3, AO) \right) \right] \quad (15.90)$$

$$\left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{c_1 e^2}{4\pi\epsilon_0 a^3}}}{m_e c^2}} + \frac{1}{2} \sqrt{\frac{\frac{c_1 e^2}{8\pi\epsilon_0 a^3} - \frac{e^2}{8\pi\epsilon_0 \left( a + \sqrt{\frac{aa_0}{2C_1 C_2}} \right)^3}}{\mu}} \right]$$

From the energy relationship given by Eq. (15.90) and the relationship between the axes given by Eqs. (15.2-15.5), the dimensions of the  $A-B$  MO can be solved. The most convenient way to solve Eq. (15.90) is by the reiterative technique using a computer.

A factor  $c_2$  of a given atom in the determination of  $c_2'$  for calculating the zero of the total  $A-B$  bond energy is typically given by Eqs. (15.62-15.65). In the case of a  $H-H$  terminal bond of an alkyl or alkenyl group,  $c_2'$  is typically the ratio of  $c_2$  of Eq. (15.62) for the  $H-H$  bond which is one and  $c_2$  of the carbon of the corresponding  $C-H$  bond:

$$c'_2 = \frac{1}{c_2(C2sp^3)} = \frac{13.605804 \text{ eV}}{E_{Coulomb}(C-H \text{ } C2sp^3)} \quad (15.91)$$

In the case of the determination of the bond angle of the *ACH* MO comprising a linear combination of *C-A*-bond and *C-H*-bond MOs where *A* and *C* are general, *C* is the central atom, and  $c_2$  for an atom is given by Eqs. (15.62-15.70),  $c'_2$  of the *A-H* terminal bond is typically the ratio of  $c_2$  of the *A* atom for the *A-H* terminal bond and  $c_2$  of the *C* atom of the corresponding *C-H* bond:

$$c'_2 = \frac{c_2(A(A-H)msp^3)}{c_2(C(C-H)msp^3)} \quad (15.92)$$

In the case of the determination of the bond angle of the *COH* MO of an alcohol comprising a linear combination of *C-O*-bond and *O-H*-bond MOs where *C*, *O*, and *H* are carbon, oxygen, and hydrogen, respectively,  $c'_2$  of the *C-H* terminal bond is typically 0.91771 since the oxygen and hydrogen atoms are at the Coulomb potential of a proton and an electron (Eqs. (1.236) and (10.162), respectively) that is energy matched to the *C2sp<sup>3</sup>* HO.

In the determination of the hybridization factor  $c'_2$  of Eq. (15.90) from Eqs. (15.62-15.70), the Coulombic energy,  $E_{Coulomb}(MO.atom,msp^3)$ , or the energy,  $E(MO.atom,msp^3)$ , the radius  $r_{A-B \text{ } AorBsp^3}$  of the *A* or *B* AO or HO of the heteroatom of the *A-B* terminal bond MO such as the *C2sp<sup>3</sup>* HO of a terminal *C-C* bond is calculated using Eq. (15.32) by considering  $\sum E_{T_{mol}}(MO,2sp^3)$ , the total energy donation to each bond with which it participates in bonding as it forms the terminal bond. The Coulombic energy  $E_{Coulomb}(MO.atom,msp^3)$  of the outer electron of the *atom msp<sup>3</sup>* shell is given by Eq. (15.19). In the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  (Eq. (15.15)) at the initial radius *r* of the AO electron. Then, the energy  $E(MO.atom,msp^3)$  of the outer electron of the *atom msp<sup>3</sup>* shell is given by the sum of  $E_{Coulomb}(MO.atom,msp^3)$  and  $E(magnetic)$  (Eq. (15.20)).

In the specific case of the terminal bonding of two carbon atoms, the  $c_2$  factor of each carbon given by Eq. (15.62) is determined using the Coulombic energy

$E_{Coulomb}(C-C\ C2sp^3)$  of the outer electron of the  $C2sp^3$  shell given by Eq. (15.19) with the radius  $r_{C-C\ C2sp^3}$  of each  $C2sp^3$  HO of the terminal  $C-C$  bond calculated using Eq. (15.32) by considering  $\sum E_{T_{mol}}(MO, 2sp^3)$ , the total energy donation to each bond with which it participates in bonding as it forms the terminal bond including the contribution of the methylene energy, 0.92918 eV (Eq. (14.513)), corresponding to the terminal  $C-C$  bond. The corresponding  $E_T(atom - atom, msp^3.AO)$  in Eq. (15.90) is  $E_T(C-C\ C2sp^3) = -1.85836\ eV$ .

In the case that the terminal atoms are carbon or other heteroatoms, the terminal bond comprises a linear combination of the HOs or AOs; thus,  $c'_2$  is the average of the hybridization factors of the participating atoms corresponding to the normalized linear sum:

$$c'_2 = \frac{1}{2}(c'_2(atom\ 1) + c'_2(atom\ 2)) \quad (15.93)$$

In the exemplary cases of  $C-C$ ,  $O-O$ , and  $N-N$  where  $C$  is carbon:

$$\begin{aligned} c'_2 &= \frac{1}{2} \left( \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-A\ A_1 AO/HO}}} + \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-A\ A_2 AO/HO}}} \right) \\ &= \frac{1}{2} \left( \frac{13.605804\ eV}{E_{Coulomb}(A-A\ A_1 AO/HO)} + \frac{13.605804\ eV}{E_{Coulomb}(A-A\ A_2 AO/HO)} \right) \end{aligned} \quad (15.94)$$

In the exemplary cases of  $C-N$ ,  $C-O$ , and  $C-S$ ,

$$c'_2 = \frac{1}{2} \left( \frac{13.605804\ eV}{E_{Coulomb}(C-B\ C2sp^3)} + c_2(C\ to\ B) \right) \quad (15.95)$$

where  $C$  is carbon and  $c_2(C\ to\ B)$  is the hybridization factor of Eqs. (15.52) and (15.84) that matches the energy of the atom  $B$  to that of the atom  $C$  in the group. For these cases, the corresponding  $E_T(atom - atom, msp^3.AO)$  term in Eq. (15.90) depends on the hybridization and bond order of the terminal atoms in the molecule, but typical values matching those used in the determination of the bond energies (Eq. (15.56)) are

$$E_T(C-O\ C2sp^3.O2p) = -1.44915\ eV; \quad E_T(C-O\ C2sp^3.O2p) = -1.65376\ eV;$$



$$\begin{aligned}
E_T(C-N \text{ } C2sp^3.N2p) &= -1.44915 \text{ eV}; & E_T(C-S \text{ } C2sp^3.S2p) &= -0.72457 \text{ eV}; \\
E_T(O-O \text{ } O2p.O2p) &= -1.44915 \text{ eV}; & E_T(O-O \text{ } O2p.O2p) &= -1.65376 \text{ eV}; \\
E_T(N-N \text{ } N2p.N2p) &= -1.44915 \text{ eV}; & E_T(N-O \text{ } N2p.O2p) &= -1.44915 \text{ eV}; \\
E_T(F-F \text{ } F2p.F2p) &= -1.44915 \text{ eV}; & E_T(Cl-Cl \text{ } Cl3p.Cl3p) &= -0.92918 \text{ eV}; \\
E_T(Br-Br \text{ } Br4p.Br4p) &= -0.92918 \text{ eV}; & E_T(I-I \text{ } I5p.I5p) &= -0.36229 \text{ eV}; \\
E_T(C-F \text{ } C2sp^3.F2p) &= -1.85836 \text{ eV}; & E_T(C-Cl \text{ } C2sp^3.Cl3p) &= -0.92918 \text{ eV}; \\
E_T(C-Br \text{ } C2sp^3.Br4p) &= -0.72457 \text{ eV}; & E_T(C-I \text{ } C2sp^3.I5p) &= -0.36228 \text{ eV}, \text{ and} \\
E_T(O-Cl \text{ } O2p.Cl3p) &= -0.92918 \text{ eV}.
\end{aligned}$$

In the case that the terminal bond is  $X-X$  where  $X$  is a halogen atom,  $c_1$  is one, and  $c'_2$  is the average (Eq. (15.93)) of the hybridization factors of the participating halogen atoms given by Eqs. (15.62-15.63) where  $E_{Coulomb}(MO.atom,msp^3)$  is determined using Eq. (15.32) and  $E_{Coulomb}(MO.atom,msp^3) = 13.605804 \text{ eV}$  for  $X = I$ . The factor  $C_1$  of Eq. (15.90) is one for all halogen atoms. The factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243). For each of the other halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $C_2$  is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with  $c_2(1)$  being that of the halogen given by Eq. (15.68) that matches the valence energy of  $X$  ( $E_1(valence)$ ) to that of the  $C2sp^3$  HO ( $E_2(valence) = -14.63489 \text{ eV}$ , Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)).  $E_T(atom-atom,msp^3.AO)$  of Eq. (15.90) is the maximum for the participating atoms which is  $-1.44915 \text{ eV}$ ,  $-0.92918 \text{ eV}$ ,  $-0.92918 \text{ eV}$ , and  $-0.33582 \text{ eV}$  for  $F$ ,  $Cl$ ,  $Br$ , and  $I$ , respectively.

Consider the case that the terminal bond is  $C-X$  where  $C$  is a carbon atom and  $X$  is a halogen atom. The factors  $c_1$  and  $C_1$  of Eq. (15.90) are one for all halogen atoms. For  $X = F$ ,  $c'_2$  is the average (Eq. (15.95)) of the hybridization factors of the participating carbon and  $F$  atoms where  $c_2$  for carbon is given by Eq. (15.62) and  $c_2$  for fluorine matched to

carbon is given by Eq. (15.70) with  $c_2(1)$  for the fluorine atom given by Eq. (15.68) that matches the valence energy of  $F$  ( $E_1(\text{valence}) = -17.42282 \text{ eV}$ ) to that of the  $C2sp^3$  HO ( $E_2(\text{valence}) = -14.63489 \text{ eV}$ , Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)). The factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243). For each of the other halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $c'_2$  is the hybridization factor of the participating carbon atom since the halogen atom is energy matched to the carbon atom.  $C_2$  of the terminal-atom bond matches that used to determine the energies of the corresponding  $C-X$ -bond MO. Then,  $C_2$  is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with  $c_2(1)$  for the halogen atom given by Eq. (15.68) that matches the valence energy of  $X$  ( $E_1(\text{valence})$ ) to that of the  $C2sp^3$  HO ( $E_2(\text{valence}) = -14.63489 \text{ eV}$ , Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)).  $E_T(\text{atom} - \text{atom}, msp^3.AO)$  of Eq. (15.90) is the maximum for the participating atoms which is  $-1.85836 \text{ eV}$ ,  $-0.92918 \text{ eV}$ ,  $-0.72457 \text{ eV}$ , and  $-0.33582 \text{ eV}$  for  $F$ ,  $Cl$ ,  $Br$ , and  $I$ , respectively.

Consider the case that the terminal bond is  $H-X$  corresponding to the angle of the atoms  $H CX$  where  $C$  is a carbon atom and  $X$  is a halogen atom. The factors  $c_1$  and  $C_1$  of Eq. (15.90) are 0.75 for all halogen atoms. For  $X = F$ ,  $c'_2$  is given by Eq. (15.69) with  $c_2$  of the participating carbon and  $F$  atoms given by Eq. (15.62) and Eq. (15.65), respectively. The factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243). For each of the other halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $c'_2$  is also given by Eq. (15.69) with  $c_2$  of the participating carbon given by Eq. (15.62) and  $c_2$  of the participating  $X$  atom given by  $c_2 = 0.91771$  (Eq. (13.430)) since the  $X$  atom is energy matched to the  $C2sp^3$  HO. In these cases,  $C_2$  is given by Eq. (15.65) for the corresponding atom  $X$  where  $C_2$  matches the energy of the atom  $X$  to that of  $H$ .

Using the distance between the two atoms  $A$  and  $B$  of the general molecular group  $ACB$  when the total energy of the corresponding  $A-B$  MO is zero, the corresponding bond angle can be determined from the law of cosines:

$$s_1^2 + s_2^2 - 2s_1s_2\cos\theta = s_3^2 \quad (15.96)$$

With  $s_1 = 2c'_{C-A}$ , the internuclear distance of the  $C-A$  bond,  $s_2 = 2c'_{C-B}$ , the internuclear distance of each  $C-B$  bond, and  $s_3 = 2c'_{A-B}$ , the internuclear distance of the two terminal atoms, the bond angle  $\theta_{\angle ACB}$  between the  $C-A$  and  $C-B$  bonds is given by

$$(2c'_{C-A})^2 + (2c'_{C-B})^2 - 2(2c'_{C-A})(2c'_{C-B})\cos\theta = (2c'_{A-B})^2 \quad (15.97)$$

$$\theta_{\angle ACB} = \cos^{-1} \left( \frac{(2c'_{C-A})^2 + (2c'_{C-B})^2 - (2c'_{A-B})^2}{2(2c'_{C-A})(2c'_{C-B})} \right) \quad (15.98)$$

Consider the exemplary structure  $C_b C_a (O_a) O_b$  wherein  $C_a$  is bound to  $C_b$ ,  $O_a$ , and  $O_b$ . In the general case that the three bonds are coplanar and two of the angles are known, say  $\theta_1$  and  $\theta_2$ , then the third  $\theta_3$  can be determined geometrically:

$$\theta_3 = 360 - \theta_1 - \theta_2 \quad (15.99)$$

In the general case that two of the three coplanar bonds are equivalent and one of the angles is known, say  $\theta_1$ , then the second and third can be determined geometrically:

$$\theta_2 = \theta_3 = \frac{(360 - \theta_1)}{2} \quad (15.100)$$

## ANGLES AND DISTANCES FOR AN MO THAT FORMS AN ISOSCELES TRIANGLE

In the general case where the group comprises three  $A-B$  bonds having  $B$  as the central atom at the apex of a pyramidal structure formed by the three bonds with the  $A$  atoms at the base in the  $xy$ -plane. The  $C_{3v}$  axis centered on  $B$  is defined as the vertical or  $z$ -axis, and any two  $A-B$  bonds form an isosceles triangle. Then, the angle of the bonds and the distances from and along the  $z$ -axis are determined from the geometrical relationships given by Eqs. (13.412-13.416):

the distance  $d_{origin-B}$  from the origin to the nucleus of a terminal  $B$  atom is given by

$$d_{\text{origin}-B} = \frac{2c'_{B-B}}{2\sin 60^\circ} \quad (15.101)$$

the height along the z-axis from the origin to the  $A$  nucleus  $d_{\text{height}}$  is given by

$$d_{\text{height}} = \sqrt{(2c'_{A-B})^2 - (d_{\text{origin}-B})^2}, \text{ and} \quad (15.102)$$

the angle  $\theta_v$  of each  $A-B$  bond from the z-axis is given by

$$\theta_v = \tan^{-1} \left( \frac{d_{\text{origin}-B}}{d_{\text{height}}} \right) \quad (15.103)$$

Consider the case where the central atom  $B$  is further bound to a fourth atom  $C$  and the  $B-C$  bond is along the z-axis. Then, the bond  $\theta_{\angle ABC}$  given by Eq. (14.206) is

$$\theta_{\angle ABC} = 180 - \theta_v \quad (15.104)$$

## DIHEDRAL ANGLE

Consider the plane defined by a general  $ACA$  MO comprising a linear combination of two  $C-A$ -bond MOs where  $C$  is the central atom. The dihedral angle  $\theta_{\angle BCI/ACA}$  between the  $ACA$ -plane and a line defined by a third bond with  $C$ , specifically that corresponding to a  $C-B$ -bond MO, is calculated from the bond angle  $\theta_{\angle ACA}$  and the distances between the  $A$ ,  $B$ , and  $C$  atoms. The distance  $d_1$  along the bisector of  $\theta_{\angle ACA}$  from  $C$  to the internuclear-distance line between  $A$  and  $A$ ,  $2c'_{A-A}$ , is given by

$$d_1 = 2c'_{C-A} \cos \frac{\theta_{\angle ACA}}{2} \quad (15.105)$$

where  $2c'_{C-A}$  is the internuclear distance between  $A$  and  $C$ . The atoms  $A$ ,  $A$ , and  $B$  define the base of a pyramid. Then, the pyramidal angle  $\theta_{\angle ABA}$  can be solved from the internuclear distances between  $A$  and  $A$ ,  $2c'_{A-A}$ , and between  $A$  and  $B$ ,  $2c'_{A-B}$ , using the law of cosines (Eq. (15.98)):

$$\theta_{\angle ABA} = \cos^{-1} \left( \frac{(2c'_{A-B})^2 + (2c'_{A-B})^2 - (2c'_{A-A})^2}{2(2c'_{A-B})(2c'_{A-B})} \right) \quad (15.106)$$

Then, the distance  $d_2$  along the bisector of  $\theta_{\angle ABA}$  from  $B$  to the internuclear-distance line  $2c'_{A-A}$ , is given by

$$d_2 = 2c'_{A-B} \cos \frac{\theta_{\angle ABA}}{2} \quad (15.107)$$

The lengths  $d_1$ ,  $d_2$ , and  $2c'_{C-B}$  define a triangle wherein the angle between  $d_1$  and the internuclear distance between  $B$  and  $C$ ,  $2c'_{C-B}$ , is the dihedral angle  $\theta_{\angle BC/ACA}$  that can be solved using the law of cosines (Eq. (15.98)):

$$\theta_{\angle BC/ACA} = \cos^{-1} \left( \frac{d_1^2 + (2c'_{C-B})^2 - d_2^2}{2d_1(2c'_{B-C})} \right) \quad (15.108)$$

## SOLUTION OF GEOMETRICAL AND ENERGY PARAMETERS OF MAJOR FUNCTIONAL GROUPS AND CORRESPONDING ORGANIC MOLECULES

The exemplary molecules given in the following sections were solved using the solutions of organic chemical functional groups as basis elements wherein the structures and energies were linearly added to achieve the molecular solutions. Each functional group can be treated as a building block to form any desired molecular solution from the corresponding linear combination. Each functional group element was solved using the atomic orbital and hybrid orbital spherical orbitals solutions bridged by molecular orbitals comprised of the  $H_2$ -type prolate spheroidal solution given in the Nature of the Chemical Bond of Hydrogen-Type Molecules section. The energy of each MO was matched at the HO or AO by matching the hybridization and total energy of the MO to the AOs and HOs. The energy  $E_{mag}$  (e.g. given by Eq. (15.58)) for a  $C2sp^3$  HO and Eq.(15.59) for an  $O2p$  AO) was subtracted for each set of unpaired electrons created by bond breakage.

The bond energy is not equal to the component energy of each bond as it exists in the molecule; although, they are close. The total energy of each group is its contribution to the total energy of the molecule as a whole. The determination of the bond energies for the creation of the separate parts must take into account the energy of the formation of any radicals and any redistribution of charge density within the pieces and the corresponding energy change with bond cleavage. Also, the vibrational energy in the transition state is dependent on the other groups that are bound to a given functional group. This will effect the functional-group energy. But, because the variations in the energy based on the balance of the

molecular composition are typically of the order of a few hundreds of electron volts at most, they were neglected.

The energy of each functional-group MO bonding to a given carbon HO is independently matched to the HO by subtracting the contribution to the change in the energy of the HO from the total MO energy given by the sum of the MO contributions and  $E(C, 2sp^3) = -14.63489 \text{ eV}$  (Eq. (13.428)). The intercept angles are determined from Eqs. (15.71-15.78) using the final radius of the HO of each atom. The final carbon-atom radius is determined using Eqs. (15.32) wherein the sum of the energy contributions of each atom to all the MOs in which it participates in bonding is determined. This final radius is used in Eqs. (15.19) and (15.20) to calculate the final valence energy of the HO of each atom at the corresponding final radius. The radius of any bonding heteroatom that contributes to a MO is calculated in the same manner, and the energy of its outermost shell is matched to that of the MO by the hybridization factor between the carbon-HO energy and the energy of the heteroatomic shell. The donation of electron density to the AOs and HOs reduces the energy. The donation of the electron density to the MO's at each AO or HO is that which causes the resulting energy to be divided equally between the participating AOs or HOs to achieve energy matching.

The molecular solutions can be used to design synthetic pathways and predict product yields based on equilibrium constants calculated from the heats of formation. New stable compositions of matter can be predicted as well as the structures of combinatorial chemistry reactions. Further important pharmaceutical applications include the ability to graphically or computationally render the structures of drugs that permit the identification of the biologically active parts of the molecules to be identified from the common spatial charge-density functions of a series of active molecules. Drugs can be designed according to geometrical parameters and bonding interactions with the data of the structure of the active site of the drug.

To calculate conformations, folding, and physical properties, the exact solutions of the charge distributions in any given molecule are used to calculate the fields, and from the fields, the interactions between groups of the same molecule or between groups on different molecules are calculated wherein the interactions are distance and relative orientation dependent. The fields and interactions can be determined using a finite-element-analysis approach of Maxwell's equations.

## AROMATIC AND HETEROCYCLIC COMPOUNDS

Aromatic and heterocyclic molecules comprise at least one of an aromatic or a cyclic conjugated alkene functional group. The latter was described in the Cyclic and Conjugated Alkenes section. The aromatic bond is uniquely stable and requires the sharing of the electrons of multiple  $H_2$ -type MOs. The results of the derivation of the parameters of the benzene molecule given in the Benzene Molecule ( $C_6H_6$ ) section can be generalized to any aromatic function group(s) of aromatic and heterocyclic compounds.

$C_6H_6$  can be considered a linear combination of three ethylene molecules wherein a  $C-H$  bond of each  $CH_2$  group of  $H_2C=CH_2$  is replaced by a  $C=C$  bond to form a six-member ring of carbon atoms. The solution of the ethylene molecule is given in the Ethylene Molecule ( $CH_2CH_2$ ) section. The radius  $r_{ethylene 2sp^3}$  ( $0.85252a_0$ ) of the  $C2sp^3$  shell of ethylene calculated from the Coulombic energy is given by Eq. (14.244). The Coulombic energy  $E_{Coulomb}(C_{ethylene}, 2sp^3)$  ( $-15.95955 eV$ ) of the outer electron of the  $C2sp^3$  shell is given by Eq. (14.245). The energy  $E(C_{ethylene}, 2sp^3)$  ( $-15.76868 eV$ ) of the outer electron of the  $C2sp^3$  shell is given by Eq. (14.246).  $E_T(C=C, 2sp^3)$  ( $-1.13380 eV$ ) (Eq. (14.247), the energy change of each  $C2sp^3$  shell with the formation of the  $C=C$ -bond MO is given by the difference between  $E(C_{ethylene}, 2sp^3)$  and  $E(C, 2sp^3)$ .  $C_6H_6$  can be solved using the same principles as those used to solve ethylene wherein the  $2s$  and  $2p$  shells of each  $C$  hybridize to form a single  $2sp^3$  shell as an energy minimum, and the sharing of electrons between two  $C2sp^3$  hybridized orbitals (HOs) to form a molecular orbital (MO) permits each participating hybridized orbital to decrease in radius and energy. Each  $2sp^3$  HO of each carbon atom initially has four unpaired electrons. Thus, the 6  $H$  atomic orbitals (AOs) of benzene contribute six electrons and the six  $sp^3$ -hybridized carbon atoms contribute twenty-four electrons to form six  $C-H$  bonds and six  $C=C$  bonds. Each  $C-H$  bond has two paired electrons with one donated from the  $H$  AO and the other from the  $C2sp^3$  HO. Each  $C=C$  bond comprises a linear combination of a factor of 0.75 of four paired electrons (three electrons) from two sets of two  $C2sp^3$  HOs of the participating carbon atoms. Each  $C-H$  and each  $C=C$  bond comprises a linear combination of one and two diatomic  $H_2$ -type MOs developed in the Nature of the Chemical Bond of Hydrogen-Type Molecules and Molecular Ions section, respectively.

Consider the case where three sets of  $C=C$ -bond MOs form bonds between the two carbon atoms of each molecule to form a six-member ring such that the six resulting bonds comprise eighteen paired electrons. Each bond comprises a linear combination of two MOs wherein each comprises two  $C2sp^3$  HOs and 75% of a  $H_2$ -type ellipsoidal MO divided between the  $C2sp^3$  HOs:

$$\left[ \begin{array}{l} 3(2 C2sp^3 + 0.75 H_2 MO) \rightarrow 3 \left( \overset{4e}{C=C} \right) - \text{ethylene-type-bond MO} \\ \rightarrow 6 \left( \overset{3e}{C=C} \right) - \text{bond MO of benzene} \end{array} \right] \quad (15.142)$$

The linear combination of each  $H_2$ -type ellipsoidal MO with each  $C2sp^3$  HO further comprises an excess 25% charge-density contribution per bond from each  $C2sp^3$  HO to the  $C=C$ -bond MO to achieve an energy minimum. Thus, the dimensional parameters of each bond  $C=C$ -bond are determined using Eqs. (15.42) and (15.1-15.5) in a form that are the same equations as those used to determine the same parameters of the  $C=C$ -bond MO of ethylene (Eqs. (14.242-14.268)) while matching the boundary conditions of the structure of benzene.

Hybridization with 25% electron donation to each  $C=C$ -bond gives rise to the  $C_{benzene}2sp^3$  HO-shell Coulombic energy  $E_{Coulomb}(C_{benzene}, 2sp^3)$  given by Eq. (14.245). To meet the equipotential condition of the union of the six  $C2sp^3$  HOs,  $c_2$  and  $C_2$  of Eq. (15.42) for the aromatic  $C=C$ -bond MO is given by Eq. (15.62) as the ratio of  $15.95955 \text{ eV}$ , the magnitude of  $E_{Coulomb}(C_{benzene}, 2sp^3)$  (Eq. (14.245)), and  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  (Eq. (1.243)):

$$C_2(benzeneC2sp^3HO) = c_2(benzeneC2sp^3HO) = \frac{13.605804 \text{ eV}}{15.95955 \text{ eV}} = 0.85252 \quad (15.143)$$

The energies of each  $C=C$  bond of benzene are also determined using the same equations as those of ethylene (Eqs. (14.251-14.253) and (14.319-14.333) with the parameters of benzene. Ethylene serves as a basis element for the  $C=C$  bonding of benzene wherein each of the six  $C=C$  bonds of benzene comprises  $(0.75)(4) = 3$  electrons according to Eq. (15.142). The total energy of the bonds of the eighteen electrons of the  $C=C$  bonds of benzene,  $E_T(C_6H_6, C=C)$ , is given by  $(6)(0.75)$  times  $E_{T+osc}(C=C)$  (Eq. (14.492)), the total energy of the  $C=C$ -bond MO of benzene including the Doppler term, minus eighteen times  $E(C, 2sp^3)$  (Eq. (14.146)), the initial energy of each  $C2sp^3$  HO of each  $C$  that forms the  $C=C$  bonds of bond order two. Thus, the total energy of the six  $C=C$  bonds of benzene with three electron per aromatic bond given by Eq. (14.493) is

$$\begin{aligned} E_T(C_6H_6, C=C) &= (6)(0.75)E_{T+osc}(C=C) - (6)(3)E(C, 2sp^3) \\ &= (6)(0.75)(-66.05796 \text{ eV}) - 18(-14.63489 \text{ eV}) \\ &= -297.26081 \text{ eV} - (-263.42798 \text{ eV}) \\ &= -33.83284 \text{ eV} \end{aligned} \quad (15.144)$$

The results of benzene can be generalized to the class of aromatic and heterocyclic compounds.  $E_{hv}$  of an aromatic bond is given by  $E_T(H_2)$  (Eqs. (11.212) and (14.486)), the maximum total energy of each  $H_2$ -type MO such that

$$\bar{E}_{osc} = n_1(\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( -31.63536831 \text{ eV} \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.145)$$

The factor of 0.75 corresponding to the three electrons per aromatic bond of bond order two given in the Benzene Molecule ( $C_6H_6$ ) section modifies Eqs. (15.52-15.56). Multiplication of



the total energy given by Eq. (15.55) by  $f_1 = 0.75$  with the substitution of Eq. (15.145) gives the total energy of the aromatic bond:

$$E_T(\text{Group}) = f_1 \left[ \begin{array}{l} E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \\ -31.63536831 \text{ eV} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e} + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r^3}} \end{array} \right] \quad (15.146)$$

The total bond energy of the aromatic group  $E_D(\text{Group})$  is the negative difference of the total energy of the group (Eq. (15.146)) and the total energy of the starting species given by the sum of  $c_4 E_{\text{initial}}(c_4 \text{ AO} / \text{HO})$  and  $c_5 E_{\text{initial}}(c_5 \text{ AO} / \text{HO})$ :

$$E_D(\text{Group}) = - \left[ \begin{array}{l} f_1 \left[ \begin{array}{l} E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \\ -31.63536831 \text{ eV} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e} + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r^3}} \end{array} \right] \\ - (c_4 E_{\text{initial}}(\text{AO} / \text{HO}) + c_5 E_{\text{initial}}(c_5 \text{ AO} / \text{HO})) \end{array} \right] \quad (15.147)$$

Since there are three electrons per aromatic bond,  $c_4$  is three times the number of aromatic bonds.

Benzene can also be considered as comprising chemical bonds between six  $CH$  radicals wherein each radical comprises a chemical bond between carbon and hydrogen atoms. The solution of the parameters of  $CH$  is given in the Hydrogen Carbide ( $CH$ ) section. Those of the benzene are given in the Benzene Molecule ( $C_6H_6$ ) section. The energy components of  $V_e$ ,  $V_p$ ,  $T$ ,  $V_m$ , and  $E_T$  are the same as those of the hydrogen carbide radical, except that  $E_T(C = C, 2sp^3) = -1.13379 \text{ eV}$  (Eq. (14.247)) is subtracted from  $E_T(CH)$  of Eq. (13.495) to match the energy of each  $C-H$ -bond MO to the decrease in the energy of the corresponding  $C2sp^3$  HO. In the corresponding generalization of the aromatic  $CH$  group, the geometrical parameters are determined using Eq. (15.42) and Eqs. (15.1-15.5) with  $E_T(\text{atom} - \text{atom}, msp^3.AO) = -1.13379 \text{ eV}$ .

The total energy of the benzene  $C-H$ -bond MO,  $E_{T_{\text{benzene}}}(C-H)$ , given by Eq. (14.467) is the sum of  $0.5 E_T(C = C, 2sp^3)$ , the energy change of each  $C2sp^3$  shell per single bond due to the decrease in radius with the formation of the corresponding  $C \equiv C$ -bond MO (Eq. (14.247)), and  $E_{T_{\text{benzene}}}(CH)$ , the  $\sigma$  MO contribution given by Eq. (14.441). In the corresponding generalization of the aromatic  $CH$  group, the energy parameters are determined using Eqs. (15.146-15.147) with  $f_1 = 1$  and  $E_T(\text{atom} - \text{atom}, msp^3.AO) = \frac{-1.13379 \text{ eV}}{2}$ . Thus, the energy

contribution to the single aromatic  $CH$  bond is one half that of the  $C=C$  double bond contribution. This matches the energies of the  $CH$  and  $C=C$  aromatic groups, conserves the electron number with the equivalent charge density as that of  $s=1$  in Eqs. (15.18-15.21), and further gives a minimum energy for the molecule. Breakage of the aromatic  $C=C$  bonds to give  $CH$  groups creates unpaired electrons in these fragments that corresponds to  $c_3 = 1$  in Eq. (15.56) with  $E_{mag}$  given by Eq. (15.58).

Each of the  $C-H$  bonds of benzene comprises two electrons according to Eq. (14.439). From the energy of each  $C-H$  bond,  $-E_{D_{benzene}}(^{12}CH)$  (Eq. (14.477)), the total energy of the twelve electrons of the six  $C-H$  bonds of benzene,  $E_T(C_6H_6, C-H)$ , given by Eq. (14.494) is

$$E_T(C_6H_6, C-H) = (6)(-E_{D_{benzene}}(^{12}CH)) = 6(-3.90454 \text{ eV}) = -23.42724 \text{ eV} \quad (15.148)$$

The total bond dissociation energy of benzene,  $E_D(C_6H_6)$ , given by Eq. (14.495) is the negative sum of  $E_T(C_6H_6, C=C)$  (Eq. (14.493)) and  $E_T(C_6H_6, C-H)$  (Eq. (14.494)):

$$\begin{aligned} E_D(C_6H_6) &= -\left(E_T(C_6H_6, C=C) + E_T(C_6H_6, C-H)\right) \\ &= -((-33.83284 \text{ eV}) + (-23.42724 \text{ eV})) \\ &= 57.2601 \text{ eV} \end{aligned} \quad (15.149)$$

Using the parameters given in Tables 15.214 and 15.216 in the general equations (Eqs. (15.42), (15.1-15.5), and (15.146-15.147)) reproduces the results for benzene given in the Benzene Molecule ( $C_6H_6$ ) section as shown in Tables 15.214 and 15.216.

The symbols of the functional groups of aromatics and hertocyclics are given in Table 15.213. The geometrical (Eqs. (15.1-15.5) and (15.42)), intercept (Eqs. (15.71-15.78)), and energy (Eqs. (15.6-15.11), (15.17-15.56), and (15.146-15.147)) parameters of aromatics and hertocyclics are given in Tables 15.214, 15.215, and 15.216, respectively. The total energy of benzene given in Table 15.217 was calculated as the sum over the integer multiple of each  $E_D(\text{Group})$  of Table 15.216 corresponding to functional-group composition of the molecule. The bond angle parameters of benzene determined using Eqs. (15.79-15.108) are given in Table 15.218.

Table 15.213. The symbols of functional groups of aromatics and hertocyclics.

Functional Group	Group Symbol
CC (aromatic bond)	$C=C$
CH (aromatic)	$CH$ (i)

Table 15.214.. The geometrical bond parameters of aromatics and hertocyclics and experimental values [1].

Parameter	$^{3e}C=C$ Group	$CH$ Group
$a (a_0)$	1.47348	1.60061
$c' (a_0)$	1.31468	1.03299
Bond Length $2c' (\square)$	1.39140	1.09327
Exp. Bond Length ( $\square$ )	1.399 (benzene)	1.101 (benzene)
$b, c (a_0)$	0.66540	1.22265
$e$	0.89223	0.64537

Table 15.216. The energy parameters (eV) of functional groups of aromatics and heterocyclics.

Parameters	$^{3e}C=C$ Group	$CH$ Group
$f_1$	0.75	1
$n_1$	2	1
$n_2$	0	0
$n_3$	0	0
$C_1$	0.5	0.75
$C_2$	0.85252	1
$c_1$	1	1
$c_2$	0.85252	0.91771
$c_3$	0	1
$c_4$	3	1
$c_5$	0	1
$C_{1o}$	0.5	0.75
$C_{2o}$	0.85252	1
$V_e (eV)$	-101.12679	-37.10024
$V_p (eV)$	20.69825	13.17125
$T (eV)$	34.31559	11.58941
$V_m (eV)$	-17.15779	-5.79470
$E_{(AO HO)} (eV)$	0	-14.63489
$\Delta E_{H_2MO} (AO HO) (eV)$	0	-1.13379

$E_T (AO/HO) (eV)$	0	-13.50110
$E_T (H_2MO) (eV)$	-63.27075	-31.63539
$E_T (atom - atom, msp^3.AO) (eV)$	-2.26759	-0.56690
$E_T (MO) (eV)$	-65.53833	-32.20226
$\omega (10^{15} \text{ rad / s})$	49.7272	26.4826
$E_K (eV)$	32.73133	17.43132
$\bar{E}_D (eV)$	-0.35806	-0.26130
$\bar{E}_{Kvib} (eV)$	0.19649 [49]	0.35532 Eq. (13.458)
$\bar{E}_{osc} (eV)$	-0.25982	-0.08364
$E_{mag} (eV)$	0.14803	0.14803
$E_T (Group) (eV)$	-49.54347	-32.28590
$E_{initial} (\epsilon_A AO/HO) (eV)$	-14.63489	-14.63489
$E_{initial} (\epsilon_S AO/HO) (eV)$	0	-13.59844
$E_D (Group) (eV)$	5.63881	3.90454

Table 15.215. The MO to HO intercept geometrical bond parameters of benzene.  $E_r$  is  $E_r(atom - atom, msp^3 AO)$ .

Bond	Atom	$E_r$ (eV) Bond 1	$E_r$ (eV) Bond 2	$E_r$ (eV) Bond 3	$E_r$ (eV) Bond 4	Final Total Energy $C2sp^3$ (eV)	$r_{initial}$ ( $a_0$ )	$r_{final}$ ( $a_0$ )
$C-H(CH)$	C	-0.85035	-0.85035	-0.56690	0	-153.88327	0.91771	0.79597
${}^{3e}C=HC_a=C$	$C_a$	-0.85035	-0.85035	-0.56690	0	-153.88327	0.91771	0.79597

Bond	$E_{Coulomb}(C2sp^3)(eV)$ Final	$E(C2sp^3)$ (eV) Final	$\theta'$ ( $^\circ$ )	$\theta_1$ ( $^\circ$ )	$\theta_2$ ( $^\circ$ )	$d_1$ ( $a_0$ )	$d_2$ ( $a_0$ )
$C-H(CH)$	-17.09334	-16.90248	74.42	105.58	38.84	1.24678	0.21379
${}^{3e}C=HC_a=C$	-17.09334	-16.90248	134.24	45.76	58.98	0.75935	0.55533

Table 15.217. The total bond energies of benzene calculated using the functional group composition and the energies of Table 15.216 compared to the experimental values [2].

Formula	Name	${}^{3e}C=C$	CH	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_6H_6$	Benzene	6	6	57.26008	57.26340	0.00006

Table 15.218. The bond angle parameters of benzene and experimental values [1].  $E_T$  is  $E_T(atom - atom, msp^3, AO)$ .

Atoms of Angle	$2c'$ Bond 1 ( $a_0$ )	$2c'$ Bond 2 ( $a_0$ )	$2c'$ Terminal Atoms ( $a_0$ )	$E_{Coulombic}$ Atom 1	Atom 1 Hybridization Designation	$E_{Coulombic}$ Atom 2	Atom 2 Hybridization Designation	$c_2$ Atom 1	$c_2$ Atom 2	$C_1$	$C_2$
$\angle CCC$ (aromatic)	2.62936	2.62936	4.5585	-17.17218	34	-17.17218	34	0.79232	0.79232	1	1
$\angle CCH$ (aromatic)											

Atoms of Angle	$c_1$	$c'_2$	$E_T$ (eV)	$\theta_v$ ( $^\circ$ )	$\theta_1$ ( $^\circ$ )	$\theta_2$ ( $^\circ$ )	Cal. $\theta$ ( $^\circ$ )	Exp. $\theta$ ( $^\circ$ )
$\angle CCC$ (aromatic)	1	0.79232	-1.85836				120.19	120 [50-52] (benzene)
$\angle CCH$ (aromatic)					120.19		119.91	120 [50-52] (benzene)

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### Software Program

The present invention relates to a system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom that is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising: processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie; and an output device in communication with the processing means for displaying said physical, Maxwellian solutions of charge, mass, and current density functions of said specie.

In one embodiment, for example, the system comprises five components: (1) the graphical user interface (GUI); (2) the routine for parsing between an input chemical structure or name and taking the input and activating a routine to call up the parts of the molecule (functional groups), which are used for determining the energies and structure to be rendered; (3) the functional-group data base that has an organization of the theoretical solutions; (4) the rendering engine, which calculates and enables manipulations of the image, such as a three-dimensional model in response to commands, as well as responds to commands for data parameters corresponding to the image such as bond energies and charge distribution and geometrical parameters; and (5) data transfer system for inputting numerical data into or out of the computational components and storage components of the main system. The system further comprises spreadsheets with solutions of the bond parameters with output in any standard spreadsheet format. The system also comprises a data-handling program to transfer data from the spreadsheets into the main program.

The output may be, for example, at least one of graphical, simulation, text, and numerical data. The output may be the calculation of at least one of: (1) a bond distance between two atoms; (2) a bond angle between three of the atoms; (3) a bond energy between two atoms; (4) orbital intercept distances and angles; and (5) charge-density functions of atomic, hybridized, and molecular orbitals, wherein the bond distance, bond angle, and bond energy are calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.

In other embodiments, the charge, current, energy, and geometrical parameters are output to be inputs to other programs that may be used in further applications. For example,

the data of heats of formation may be input to another program to be used to predict stability (existence of compounds) equilibrium constants and to predict synthetic pathways. That is, a novel composition of matter may be discovered by calculating at least one of a bond distance between two of the atoms, a bond angle between three of the atoms, and a bond energy between two of the atoms, orbital intercept distances and angles, charge-density functions of atomic, hybridized, and molecular orbitals, the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration. The charge and current density functions may be used to predict the electric and magnetic fields of the species to determine other properties due to the interaction of the fields between species. These fields and the predictions of field interactions may be computed using Maxwell's equations. In one embodiment, finite-element analysis is used to predict or calculate the interaction and resulting properties, such as the freezing point, boiling point, density, viscosity, and refractive index. Furthermore, the output data can be used to give thermodynamic, spectroscopic, and other properties, aid in drug design and other applications with or without direct visualization. Furthermore, the data can be input into other programs of the system, which calculate thermodynamic and other properties, or performs a simulation, such as a chemical reaction or molecular dynamics.

The output data may be used to predict a composition of matter comprising a plurality of atoms, the improvement comprising a novel property or use discovered by calculation of at least one of a bond distance between two of the atoms, a bond angle between three of the atoms, and a bond energy between two of the atoms, orbital intercept distances and angles, charge-density functions of atomic, hybridized, and molecular orbitals, the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration. The novel property, for example, may be a new pharmaceutical use, or stability at room temperature of a novel arrangement of atoms or ions.

In one embodiment, the output device of the system is a display that displays at least one of visual or graphical media. The display may be at least one of static or dynamic. At least one of vibration, rotation, and translation may be displayed. The displayed information may be used for at least one of modeling reactivity, predicting physical properties, and aiding in drug and material design. The output device may be a monitor, video projector, printer, or

one-, two- or three-dimensional rendering device. The displayed information may be used to model other molecules and provides utility to anticipate their reactivity and physical properties. Additionally, data may be output and used in the same and additional applications as the rendered models and representations of the calculated physical solutions. The processing means of the system may be a general-purpose computer. The general-purpose computer may comprise a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage device, an input means. The input means may comprise a serial port, USB port, microphone input, camera input, keyboard or mouse. The processing means comprises a special purpose computer or other hardware system. The system may comprise computer program products such as computer readable medium having embodied therein program code means. The computer readable media may be any available media which can be accessed by a general purpose or special purpose computer. The computer readable media may comprise, for example, at least one of RAM, ROM, EPROM, CD ROM, DVD or other optical disk storage, magnetic disk storage or other magnetic storage devices, or any other medium that can embody the desired program code means and which can be accessed by a general purpose or special purpose computer. The program code means may comprise executable instructions and data, which cause a general purpose computer or special purpose computer to perform a certain function of a group of functions. Commercial examples of suitable program language includes, for example, C++, C, JAVA, FORTRAN, Python and Assembly Languages, programmed with an algorithm based on the physical solutions, and the computer may be a PC, mainframe, supercomputer, or cluster of computers. Commercial examples of suitable programs include, for example, APIs like OpenGL, DirectX, FOX GUI toolkit, and Qt. This program may be developed to run on at least one of operating systems like Windows XP, Windows 2000, Windows Vista, MAC OS, MAC OS X, Linux, Unix, Irix and other Unix-type operating systems.

Millsian software is designed to render 3-D models of molecules, molecular ions, molecular radicals, functional groups thereof, and related structure and property information and produce useful data output and application of the parameters of these species, wherein the nature of their bound electrons and chemical bonds are solved using Dr. Randell L. Mills' Classical Quantum Mechanics theory described in the reference: R. L. Mills, "The Grand Unified Theory of Classical Quantum Mechanics", June 2006 Edition, Cadmus Professional Communications-Science Press Division, Ephrata, PA, ISBN 0963517171, Library of Congress Control Number 2005936834; posted at

<http://www.blacklightpower.com/bookdownload.shtml>, which is incorporated by this reference in its entirety. Figure 76 provides a flow chart diagram, which is an example of a software system that can be utilized for this purpose, which example is not intended to limit the scope of the disclosed inventions. The main parts of this exemplary software system illustrated in Figure 1 will now be further explained:

**Start:** A user can start the program by running an executable program file. That might be done, for example, by double clicking the program icon on a Windows-based operating system, or typing the name of the executable file on the command line and pressing the 'Enter' key on a Linux or Unix operating system. The program initially starts by reading data files located in specific directories. The names of those directories and locations are fixed according to the type and format of the data files.

**Data files:** There are two types of data files used in the software system: functional group data files and molecule data files. Functional group data files contain information about various functional groups. Functional groups are the basic bonding elements or units that each typically comprise an atom, or at least two atoms bound together as found within a molecule (e.g. -Cl, C=C, C=O, CH<sub>3</sub>). Functional groups typically dictate or define properties and structure of the molecule. Similar functional groups in different molecules typically react in similar ways when subjected to a particular set of reaction conditions. Molecule data files contain information about molecules, molecular ions, and molecular radicals. These data files are processed according to their file formats.

**File formats:** Millsian software employs two kinds of file formats for storing information about the structure, energies and names of molecules and functional groups: raw-data format and hierarchical format. In a raw-data file, all information is stored as is, below the header describing the type of information. As shown in the Table below, for example, the names of the molecule or functional group are listed below the #NAMES header. The names and positions of the atoms are listed below the #ATOMS header, and so on.

```

#NAMES
CH3
Alkane CH3

#SMILES
C-

#ATOMS
1      C      0      0      0
2      H      1.9775 -0.698 0
3      H      -0.9888      -0.698 1.712
4      H      -0.9888      -0.698 -1.712

#AO
1      1 1s    0.171 2
2      1 2sp3  0.864 -1

#BONDS
1      1 2      1      1.649
2      1 3      1      1.649
3      1 4      1      1.649

#BONDAXES
1      1      1      90      0      0

#DATA
RCH bond angle: 109.44°
CH bond length: 2.097 a
HFORM: 12.492

```

Most of the functional groups files and some simple molecule files are stored in raw data format. The other file format used with the Millsian software system, the hierarchical file format, represents the information in a graph style, in which nodes are connected to other nodes through links. This format is designed to construct molecules by attaching different functional groups in a desired manner. Using this file format, the user can construct complex molecules built from solved functional groups.

For example, as shown in the Table below, the pentane data file includes a #GROUPS header below which is list all of the functional groups that form a part of the pentane molecule. Under the #GROUP\_LINKS header is information about how these functional groups are connected to each other to construct pentane.



```

#NAMES
Pentane

#SMILES
CCCCC

#GROUPS
1      C-
2      -C-
3      -C-
4      -C-
5      C-

#GROUP_LINKS
1      1 1    2 1    180
2      2 2    3 1    180
3      3 2    4 1    180
4      4 2    5 1    180

```

Processing data files: As further shown in the flow diagram of Figure 1 for the exemplary Millsian software system, the program first processes the functional group data file and constructs the functional-group objects, which are complete 3-D representations of the functional groups and their related information supplied in the corresponding file. These objects are then ready to be visually displayed through use of a molecule viewer. Next, the program processes the molecule data file. If the molecule data file is in raw-data format, then the program makes a molecule object directly from it. If the file is in hierarchical format, then the program calculates geometric parameters from listed functional groups. The program stores all functional-group objects and molecule objects using internal data structures.

Visualization/ User Interactions: As shown in Figures 2 and 3, the molecule viewer displays the functional-group objects and molecule objects and provides basic interaction capabilities with the displayed objects, such as rotating, scaling, and moving the objects. The molecule viewer also provides other visualization options, such as viewing molecules in wire frame mode, viewing coordinate axes, and changing of the transparency and lighting. The user, for example, can also select parts of a molecule for visualization, like a nucleus, atomic orbital, molecular orbital, or bond axis. The viewer also includes a drop down information window, which provides, for example, related information about molecules, such as bond angles, component functional groups, and total heat of formation. In one embodiment, a user can create new molecules by joining functional groups. For this purpose, the user can select a

first functional group. Next, the user can select an open bond from the functional group where the user desires to attach another group. Next, the user can select another or the same functional group, followed by selecting an open bond from the other group. The user can join the two selected functional groups at the selected open bonds by clicking on 'Join Groups'. This method of joining functional groups at open bonds can be repeated to form the desired molecule.

SMILES input: The Simplified Molecular Input Line Entry Specification or SMILES is a specification for unambiguously describing the structure of chemical molecules using short ASCII strings. Through the user interface, a user can enter SMILES to construct molecules, provided the new molecule comprises functional groups that are in the database. Once a SMILES is entered, a parser reads in and breaks it down into component functional groups. The software system then attaches the component functional groups to create the new molecule object, which can then be viewed using the molecule viewer.

While the claimed invention has been described in detail and with reference to specific embodiments thereof, it will be apparent to one of ordinary skill in the art that various changes and modifications can be made to the claimed invention without departing from the spirit and scope thereof.

## CLAIM:

1. A system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom that is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising:  
    processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie; and  
    an output device in communication with the processing means for displaying said physical, Maxwellian solutions of charge, mass, and current density functions of said specie.
2. The system of claim 1 wherein the output device is a display that displays at least one of visual or graphical media.
3. The system of claim 2 wherein the display is at least one of static or dynamic.
4. The system of claim 3 wherein at least one of vibration and rotation is be displayed.
5. The system of claim 4 wherein displayed information is used to model reactivity and physical properties.
6. The system of claim 5, wherein the output device is a monitor, video projector, printer, or three-dimensional rendering device.
7. The system of claim 6 wherein displayed information is used to model other species and provides utility to anticipate their reactivity and physical properties.
8. The system of claim 7 wherein the processing means is a general purpose computer.
9. The system of claim 8 wherein the general purpose computer comprises a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage device, an input means.

10. The system of claim 9, wherein the input means comprises a serial port, usb port, microphone input, camera input, keyboard or mouse.
11. The system of claim 10 wherein the processing means comprises a special purpose computer or other hardware system.
12. The system of claim 11 further comprising computer program products.
13. The system of claim 12 further comprising computer readable medium having embodied therein program code means.
14. The system of claim 13 wherein the computer readable media is any available media which can be accessed by a general purpose or special purpose computer.
15. The system of claim 14 wherein the computer readable media comprises at least one of RAM, ROM, EPROM, CD ROM, DVD or other optical disk storage, magnetic disk storage or other magnetic storage devices, or any other medium which can embody the desired program code means and which can be accessed by a general purpose or special purpose computer.
16. The system of claim 15 wherein the program code means comprises executable instructions and data which cause a general purpose computer or special purpose computer to perform a certain function of a group of functions.
17. The system of claim 16 wherein the program code is Mathematica programmed with an algorithm based on the physical solutions, and the computer is a PC.
18. The system of claim 17 wherein the algorithm is  $\text{ParametricPlot3D}[\{2*\text{Sqrt}[1-z*z]*\text{Cos}[u], \text{Sqrt}[(1-z*z)]*\text{Sin}[u], z\}, \{u, 0, 2*\text{Pi}\}, \{z, -1, .9999\}]$ , and the rendering is viewed from different perspectives.

19. The system of claim 18 wherein the algorithms for viewing from different perspectives comprises Show[Out[1], ViewPoint->{x,y,z}] where x, y, and z are Cartesian coordinates.
20. The system of claim 19 wherein the physical, Maxwellian solutions of the charge, mass, and current density functions of said specie comprises a solution of the classical wave equation  $\left[ \nabla^2 - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right] \rho(r, \theta, \phi, t) = 0$  which is the equation of motion of the charge.
21. The system of claim 20 wherein the boundary constraint of the wave equation solution is nonradiation according to Maxwell's equations.
22. The system according to claim 1, wherein the force generalized constant  $k'$  of a  $H_2$ -type ellipsoidal MO due to the equivalent of two point charges at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\epsilon_0} \quad (15.1)$$

where  $C_1$  is the fraction of the  $H_2$ -type ellipsoidal molecular orbital basis function of a chemical bond of the specie and  $C_2$  is the factor that results in an equipotential energy match of the participating at least two molecular or atomic orbitals of the chemical bond.

23. The system according to claim 1, wherein the distance from the origin of the MO to each focus  $c'$  is given by:

$$c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{a a_0}{2C_1 C_2}} \quad (15.2)$$

the internuclear distance is

$$2c' = 2 \sqrt{\frac{a a_0}{2C_1 C_2}} \quad (15.3)$$

the length of the semiminor axis of the prolate spheroidal MO  $b = c$  is given by

$$b = \sqrt{a^2 - c'^2} \quad (15.4)$$

and, the eccentricity,  $e$ , is

$$e = \frac{c'}{a} \quad (15.5).$$

24. The system according to claim 23, wherein a potential energy of the electrons in the central field of the nuclei at the foci is

$$V_e = n_1 c_1 c_2 \frac{-2e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.6)$$

where  $n_1$  is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

25. The system according to claim 1, wherein the potential energy of the two nuclei is

$$V_p = n_1 \frac{e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \quad (15.7).$$

26. The system according to claim 1, wherein the kinetic energy of the electrons is

$$T = n_1 c_1 c_2 \frac{\hbar^2}{2m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.8)$$

where  $n_1$  is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

27. The system according to claim 1, wherein the energy,  $V_m$ , of the magnetic force between the electrons is

$$V_m = n_1 c_1 c_2 \frac{-\hbar^2}{4m_e a \sqrt{a^2 - b^2}} \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} \quad (15.9)$$

where  $n_1$  is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

28. The system according to claim 1, wherein total energy of the  $H_2$ -type prolate spheroidal MO,  $E_T(H_2MO)$ , is given by the sum of the energy terms:

$$E_T(H_2MO) = V_e + T + V_m + V_p \quad (15.10)$$

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] \end{aligned} \quad (15.11)$$

where  $n_1$  is the number of equivalent bonds of the MO for functional groups and in the case of independent MOs not in contact with the bonding atoms, the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor, which is 1 for a single bond, 4 for an independent double bond and 9 for an independent triplet bond.

29. The system according to claim 1, wherein the total energy  $E_T(atom, msp^3)$  ( $m$  is the integer of the valence shell) of the AO electrons and the hybridized shell is given by the sum of energies of successive ions of the atom over the  $n$  electrons comprising total electrons of the at least one AO shell according to the formula:

$$E_T(atom, msp^3) = -\sum_{m=1}^n IP_m \quad (15.12)$$

where  $IP_m$  is the  $m$ th ionization energy (positive) of the atom.

30. The system according to claim 29, wherein the radius  $r_{msp^3}$  of the hybridized shell is given by:

$$r_{msp^3} = \sum_{q=Z-n}^{Z-1} \frac{-(Z-q)e^2}{8\pi\epsilon_0 E_T(atom, msp^3)} \quad (15.13).$$

31. The system according to claim 29, wherein the Coulombic energy  $E_{Coulomb}(atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by

$$E_{Coulomb}(atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} \quad (15.14).$$

32. The system of claim 31, wherein in the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  at the initial radius  $r$  of the AO electron:

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} = \frac{8\pi\mu_0 \mu_B^2}{r^3} \quad (15.15)$$

then, the energy  $E(atom, msp^3)$  of the outer electron of the  $atom msp^3$  shell is given by the sum of  $E_{Coulomb}(atom, msp^3)$  and  $E(magnetic)$ :

$$E(atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \quad (15.16).$$

33. The system according to claim 29, wherein the total energy  $E_T(mol.atom, msp^3)$  ( $m$  is the integer of the valence shell) of the HO electrons is given by the sum of energies of successive ions of the atom over the  $n$  electrons comprising total electrons of the at least one initial AO shell and the hybridization energy:

$$E_T(mol.atom, msp^3) = E(atom, msp^3) - \sum_{m=2}^n IP_m \quad (15.17)$$

where  $IP_m$  is the  $m$ th ionization energy (positive) of the atom and the sum of  $-IP_1$  plus the hybridization energy is  $E(atom, msp^3)$ .

34. The system of claim 33, wherein the radius  $r_{msp^3}$  of the hybridized shell is given by:



$$r_{msp^3} = \left( \sum_{q=Z-n}^{Z-1} (Z-q) - s(0.25) \right) \frac{-e^2}{8\pi\epsilon_0 E_T(mol.atom, msp^3)} \quad (15.18)$$

where  $s = 1, 2, 3$  for a single, double, and triple bond, respectively.

35. The system of claim 34, wherein the Coulombic energy  $E_{Coulomb}(mol.atom, msp^3)$  of the outer electron of the  $atom\ msp^3$  shell is given by

$$E_{Coulomb}(mol.atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} \quad (15.19).$$

36. The system of claim 35, wherein in the case that during hybridization at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  at the initial radius  $r$  of the AO electron given by Eq. (15.15). Then, the energy  $E(mol.atom, msp^3)$  of the outer electron of the  $atom\ msp^3$  shell is given by the sum of  $E_{Coulomb}(mol.atom, msp^3)$  and  $E(magnetic)$ :

$$E(mol.atom, msp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{msp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} \quad (15.20)$$

$E_T(atom - atom, msp^3)$ , the energy change of each  $atom\ msp^3$  shell with the formation of the atom-atom-bond MO is given by the difference between  $E(mol.atom, msp^3)$  and  $E(atom, msp^3)$ :

$$E_T(atom - atom, msp^3) = E(mol.atom, msp^3) - E(atom, msp^3) \quad (15.21).$$

37. The system of claim 31, wherein  $E_{Coulomb}(mol.atom, msp^3)$  is one of:

$E_{Coulomb}(C_{ethylene}, 2sp^3)$ ,  $E_{Coulomb}(C_{ethane}, 2sp^3)$ ,  $E_{Coulomb}(C_{acetylene}, 2sp^3)$ , and  $E_{Coulomb}(C_{alkane}, 2sp^3)$ ;

$E_{Coulomb}(atom, msp^3)$  is one of  $E_{Coulomb}(C, 2sp^3)$  and  $E_{Coulomb}(Cl, 3sp^3)$ ;

$E(mol.atom, msp^3)$  is one of  $E(C_{ethylene}, 2sp^3)$ ,  $E(C_{ethane}, 2sp^3)$ ,

$$E(C_{\text{acetylene}}, 2sp^3) E(C_{\text{alkane}}, 2sp^3);$$

$$E(\text{atom}, msp^3) \text{ is one of } E(C, 2sp^3) \text{ and } E(Cl, 3sp^3);$$

$$E_T(\text{atom} - \text{atom}, msp^3) \text{ is one of } E(C - C, 2sp^3), E(C = C, 2sp^3), \text{ and}$$

$$E(C \equiv C, 2sp^3);$$

$$\text{atom } msp^3 \text{ is one of } C2sp^3, Cl3sp^3$$

$$E_T(\text{atom} - \text{atom}(s_1), msp^3) \text{ is } E_T(C - C, 2sp^3) \text{ and } E_T(\text{atom} - \text{atom}(s_2), msp^3) \text{ is}$$

$$E_T(C = C, 2sp^3), \text{ and}$$

$$r_{msp^3} \text{ is one of } r_{C2sp^3}, r_{\text{ethane}2sp^3}, r_{\text{ethylene}2sp^3}, r_{\text{acetylene}2sp^3}, r_{\text{alkane}2sp^3}, \text{ and } r_{Cl3sp^3}.$$

In the case of the  $C2sp^3$  HO, the initial parameters (Eqs. (14.142-14.146)) are

$$r_{2sp^3} = \sum_{n=2}^5 \frac{(Z-n)e^2}{8\pi\epsilon_0 (e148.25751 \text{ eV})} = \frac{10e^2}{8\pi\epsilon_0 (e148.25751 \text{ eV})} = 0.91771a_0 \quad (15.22)$$

$$E_{\text{Coulomb}}(C, 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} = \frac{-e^2}{8\pi\epsilon_0 0.91771a_0} = -14.82575 \text{ eV} \quad (15.23)$$

$$E(\text{magnetic}) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} = \frac{8\pi\mu_0 \mu_B^2}{(0.84317a_0)^3} = 0.19086 \text{ eV} \quad (15.24)$$

$$\begin{aligned} E(C, 2sp^3) &= \frac{-e^2}{8\pi\epsilon_0 r_{2sp^3}} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (r_3)^3} \\ &= -14.82575 \text{ eV} + 0.19086 \text{ eV} \\ &= -14.63489 \text{ eV} \end{aligned} \quad (15.25)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

38. The system of claim 37, wherein

$$\sum_{q=Z-n}^{Z-1} (Z-q) = 10 \quad (15.26)$$

Equations (14.147) and (15.17) give

$$E_T(\text{mol.atom}, msp^3) = E_T(C_{\text{ethane}}, 2sp^3) = -151.61569 \text{ eV} \quad (15.27)$$

and using Eqs. (15.18-15.28), the final values of  $r_{C2sp^3}$ ,  $E_{Coulomb}(C2sp^3)$ , and  $E(C2sp^3)$ , and the resulting  $E_T\left(C - C^{BO}, C2sp^3\right)$  of the MO due to charge donation from the HO to the MO where  $C - C^{BO}$  refers to the bond order of the carbon-carbon bond for different values of the parameter  $s$  are given in Table 15.1.

Table 15.1:

MO Bond Order (BO)	$s$ 1	$s$ 2	$r_{C2sp^3}(a_0)$ Final	$E_{Coulomb}(C2sp^3)(eV)$ Final	$E(C2sp^3)$ (eV) Final	$E_T\left(C - C^{BO}, C2sp^3\right)$ (eV)
I	1	0	0.87495	-15.55033	-15.35946	-0.72457
II	2	0	0.85252	-15.95955	-15.76868	-1.13379
III	3	0	0.83008	-16.39089	-16.20002	-1.56513
IV	4	0	0.80765	-16.84619	-16.65532	-2.02043

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

39. The system of claim 33, wherein a minimum-energy bond with the constraint that it must meet the energy matching condition for all MOs at all HOs or AOs, the energy

$E(mol.atom,msp^3)$  of the outer electron of the  $atom msp^3$  shell of each bonding atom is the average of  $E(mol.atom,msp^3)$  for two different values of  $s$ :

$$E(mol.atom,msp^3) = \frac{E(mol.atom(s_1),msp^3) + E(mol.atom(s_2),msp^3)}{2} \quad (15.28).$$

40. The system of claim 39, wherein in the case,  $E_T(atom - atom,msp^3)$ , the energy change of each  $atom msp^3$  shell with the formation of each atom-atom-bond MO, is average for two different values of  $s$ :

$$E_T(\text{atom} - \text{atom}, msp^3) = \frac{E_T(\text{atom} - \text{atom}(s_1), msp^3) + E_T(\text{atom} - \text{atom}(s_2), msp^3)}{2} \quad (15.29).$$

41. The system of claim 39, wherein a first MO and its HOs comprising a linear combination of bond orders and a second MO that shares a HO with the first. In addition to the mutual HO, the second MO comprises another AO or HO having a single bond order or a mixed bond order, in order for the two MOs to be energy matched, the bond order of the second MO and its HOs or its HO and AO is a linear combination of the terms corresponding to the bond order of the mutual HO and the bond order of the independent HO or AO, and in general,  $E_T(\text{atom} - \text{atom}, msp^3)$ , the energy change of each  $\text{atom } msp^3$  shell with the formation of each atom-atom-bond MO, is a weighted linear sum for different values of  $s$  that matches the energy of the bonded MOs, HOs, and AOs:

$$E_T(\text{atom} - \text{atom}, msp^3) = \sum_{n=1}^N c_{s_n} E_T(\text{atom} - \text{atom}(s_n), msp^3) \quad (15.30)$$

where  $c_{s_n}$  is the multiple of the BO of  $s_n$ . The radius  $r_{msp^3}$  of the  $\text{atom } msp^3$  shell of each bonding atom is given by the Coulombic energy using the initial energy  $E_{Coulomb}(\text{atom}, msp^3)$  and  $E_T(\text{atom} - \text{atom}, msp^3)$ , the energy change of each  $\text{atom } msp^3$  shell with the formation of each atom-atom-bond MO:

$$r_{msp^3} = \frac{-e^2}{8\pi\epsilon_0 a_0 (E_{Coulomb}(\text{atom}, msp^3) + E_T(\text{atom} - \text{atom}, msp^3))} \quad (15.31)$$

where  $E_{Coulomb}(C2sp^3) = -14.825751 \text{ eV}$ .

42. The system of claim 41, wherein the Coulombic energy  $E_{Coulomb}(\text{mol. atom}, msp^3)$  of the outer electron of the  $\text{atom } msp^3$  shell is given by Eq. (15.19).

43. The system of claim 42, wherein in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(\text{magnetic})$  (Eq. (15.15)) at the initial radius  $r$  of the AO electron. Then, the energy  $E(\text{mol. atom}, msp^3)$  of the outer

electron of the *atom msp<sup>3</sup>* shell is given by the sum of  $E_{Coulomb}(mol.atom, msp^3)$  and  $E(magnetic)$  (Eq. (15.20)).

44. The system of claim 42, wherein,  $E_t(atom - atom, msp^3)$ , the energy change of each *atom msp<sup>3</sup>* shell with the formation of the atom-atom-bond MO is given by the difference between  $E(mol.atom, msp^3)$  and  $E(atom, msp^3)$  given by Eq. (15.21).

45. The system of claim 44, wherein using the equation (15.23) for  $E_{Coulomb}(C, 2sp^3)$  in equation (15.31), the single bond order energies given by Eqs. (15.18-15.27) and shown in Table 15.1, and the linear combination energies (Eqs. (15.28-15.30)), the parameters of linear combinations of bond orders and linear combinations of mixed bond orders are given in Table 15.2, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

46. The system of claim 29, wherein the radius  $r_{mol2sp^3}$  of the  $C2sp^3$  HO of a carbon atom of a given specie is calculated using Eq. (14.514) by considering  $\sum E_{T_{mol}}(MO, 2sp^3)$ , the total energy donation to each bond with which it participates in bonding.

47. The system of claim 1, wherein equation for the radius is given by

$$r_{mol2sp^3} = \frac{-e^2}{8\pi\epsilon_0 \left( E_{Coulomb}(C, 2sp^3) + \sum E_{T_{mol}}(MO, 2sp^3) \right)} \quad (15.32).$$

$$= \frac{e^2}{8\pi\epsilon_0 \left( e14.825751 \text{ eV} + \sum |E_{T_{mol}}(MO, 2sp^3)| \right)}$$

48. The system of 29, wherein the Coulombic energy  $E_{Coulomb}(mol.atom, msp^3)$  of the outer electron of the *atom msp<sup>3</sup>* shell is given by Eq. (15.19).

49. The system of claim 29, in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(\text{magnetic})$  (Eq. (15.15)) at the initial radius  $r$  of the AO electron. Then, the energy  $E(\text{mol. atom}, msp^3)$  of the outer electron of the *atom msp<sup>3</sup>* shell is given by the sum of  $E_{\text{Coulomb}}(\text{mol. atom}, msp^3)$  and  $E(\text{magnetic})$  (Eq. (15.20)).
50. The system of claim 49, wherein for the  $C2sp^3$  HO of each methyl group of an alkane contributes  $-0.92918 \text{ eV}$  (Eq. (14.513)) to the corresponding single  $C-C$  bond; the corresponding  $C2sp^3$  HO radius is given by Eq. (14.514). The  $C2sp^3$  HO of each methylene group of  $C_nH_{2n+2}$  contributes  $-0.92918 \text{ eV}$  to each of the two corresponding  $C-C$  bond MOs, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.
51. The system of claim 50, wherein the radius (Eq. (15.32)), the Coulombic energy (Eq. (15.19)), and the energy (Eq. (15.20)) of each alkane methylene group are

$$\begin{aligned}
 r_{\text{alkaneC}_{\text{methylene}} 2sp^3} &= \frac{-e^2}{8\pi\epsilon_0 \left( E_{\text{Coulomb}}(C, 2sp^3) + \sum E_{T_{\text{alkane}}}(\text{methylene } C-C, 2sp^3) \right)} \\
 &= \frac{e^2}{8\pi\epsilon_0 (e14.825751 \text{ eV} + e0.92918 \text{ eV} + e0.92918 \text{ eV})} \\
 &= 0.81549a_0
 \end{aligned}$$

(15.33)

$$E_{\text{Coulomb}}(C_{\text{methylene}} 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 (0.81549a_0)} = -16.68412 \text{ eV} \quad (15.34)$$

$$E(C_{\text{methylene}} 2sp^3) = \frac{-e^2}{8\pi\epsilon_0 (0.81549a_0)} + \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 (0.84317a_0)^3} = -16.49325 \text{ eV} \quad (15.35)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

52. The system of claim 51, wherein in the determination of the parameters of functional groups, heteroatoms bonding to  $C2sp^3$  HOs to form MOs are energy matched to the

$C2sp^3$  HOs, the radius and the energy parameters of a bonding heteroatom are given by the same equations as those for  $C2sp^3$  HOs.

53. The system of claim 52, wherein using Eqs. (15.15), (15.19-15.20), (15.24), and (15.32) in a generalized fashion, the final values of the radius of the HO or AO,  $r_{Atom.HO.AO}$ ,

$E_{Coulomb}(mol.atom,msp^3)$ , and  $E(C_{mol}2sp^3)$  are calculated using  $\sum E_{T_{group}}(MO,2sp^3)$ ,

the total energy donation to each bond with which an atom participates in bonding

corresponding to the values of  $E_T\left(C^{BO}-C,C2sp^3\right)$  of the MO due to charge donation

from the AO or HO to the MO given in Tables 15.1 and 15.2 and the final values of

$r_{Atom.HO.AO}$ ,  $E_{Coulomb}(mol.atom,msp^3)$ , and  $E(C_{mol}2sp^3)$  calculated using the values of

$E_T\left(C^{BO}-C,C2sp^3\right)$  given in Tables 15.1 and 15.2 are shown in Tables 15.3A and 15.3B

in the specification, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

54. The system of claim 53, wherein the energy of the MO is matched to each of the participating outermost atomic or hybridized orbitals of the bonding atoms wherein the energy match includes the energy contribution due to the AO or HO's donation of charge to the MO.

55. The system of claim 54, wherein the force constant  $k'$  (Eq. (15.1)) is used to determine the ellipsoidal parameter  $c'$  (Eq. (15.2)) of the each  $H_2$ -type-ellipsoidal-MO in terms of the central force of the foci,  $c'$  is substituted into the energy equation (from Eq. (15.11)) which is set equal to  $n_1$  times the total energy of  $H_2$  where  $n_1$  is the number of equivalent bonds of the MO and the energy of  $H_2$ ,  $-31.63536831 \text{ eV}$ , Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

56. The system of claim 55, wherein the energy equation and the relationship between the axes, the dimensions of the MO are solved, the energy equation has the semimajor axis  $a$  as its only parameter, the solution of the semimajor axis  $a$  allows for the solution of the other axes of each prolate spheroid and eccentricity of each MO (Eqs. (15.3-15.5)), and the parameter solutions then allow for the component and total energies of the MO to be determined.

57. The system of claim 1, wherein the total energy,  $E_T(H_2MO)$ , is given by the sum of the energy terms (Eqs. (15.6-15.11)) plus  $E_T(AO/HO)$ :

$$E_T(H_2MO) = V_e + T + V_m + V_p + E_T(AO/HO) \quad (15.36)$$

$$\begin{aligned} E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] + E_T(AO/HO) \\ &= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] + E_T(AO/HO) \end{aligned} \quad (15.37)$$

where  $n_1$  is the number of equivalent bonds of the MO,  $c_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of a chemical bond of the group,  $c_2$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of each chemical bond, and  $E_T(AO/HO)$  is the total energy comprising the difference of the energy  $E(AO/HO)$  of at least one atomic or hybrid orbital to which the MO is energy matched and any energy component  $\Delta E_{H_2MO}(AO/HO)$  due to the AO or HO's charge donation to the MO.

58. The system of claim 57, wherein

$$E_T(AO/HO) = E(AO/HO) - \Delta E_{H_2MO}(AO/HO) \quad (15.38)$$

59. The system of claim 58, wherein as specific examples,  $E_T(AO/HO)$  is one from the group of

$$E_T(AO/HO) = E(O2p \text{ shell}) = -E(\text{ionization}; O) = -13.6181 \text{ eV};$$

$$E_T(AO/HO) = E(N2p \text{ shell}) = -E(\text{ionization}; N) = -14.53414 \text{ eV};$$



$$\begin{aligned}
E_T(AO/HO) &= E(C, 2sp^3) = -14.63489 \text{ eV}; \\
E_T(AO/HO) &= E_{Coulomb}(Cl, 3sp^3) = -14.60295 \text{ eV}; \\
E_T(AO/HO) &= E(\text{ionization}; C) + E(\text{ionization}; C^+); \\
E_T(AO/HO) &= E(C_{ethane}, 2sp^3) = -15.35946 \text{ eV}; \\
E_T(AO/HO) &= +E(C_{ethylene}, 2sp^3) - E(C_{ethylene}, 2sp^3); \\
E_T(AO/HO) &= E(C, 2sp^3) - 2E_T(C=C, 2sp^3) = -14.63489 \text{ eV} - (-2.26758 \text{ eV}); \\
E_T(AO/HO) &= E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) - E(C_{acetylene}, 2sp^3) = 16.20002 \text{ eV}; \\
E_T(AO/HO) &= E(C, 2sp^3) - 2E_T(C \equiv C, 2sp^3) = -14.63489 \text{ eV} - (-3.13026 \text{ eV}); \\
E_T(AO/HO) &= E(C_{benzene}, 2sp^3) - E(C_{benzene}, 2sp^3); \\
E_T(AO/HO) &= E(C, 2sp^3) - E_T(C=C, 2sp^3) = -14.63489 \text{ eV} - (-1.13379 \text{ eV}), \text{ and} \\
E_T(AO/HO) &= E(C_{alkane}, 2sp^3) = -15.56407 \text{ eV}, \text{ wherein the calculated and measured} \\
&\text{values and constants recited in the equations herein can be adjusted, for example, up to } \pm \\
&10\%, \text{ if desired.}
\end{aligned}$$

60. The system of claim 1, wherein to solve the bond parameters and energies,

$$\begin{aligned}
c' &= a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}} \text{ (Eq. (15.2)) is substituted into } E_T(H_2MO) \text{ to give} \\
E_T(H_2MO) &= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{a^2 - b^2}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{a^2 - b^2}}{a - \sqrt{a^2 - b^2}} - 1 \right] + E_T(AO/HO) \\
&= -\frac{n_1 e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + c'}{a - c'} - 1 \right] + E_T(AO/HO) \\
&= -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(AO/HO) \\
(15.39)
\end{aligned}$$

wherein the total energy is set equal to  $E(\text{basis energies})$  which in the most general case is given by the sum of a first integer  $n_1$  times the total energy of  $H_2$  minus a second integer  $n_2$

times the total energy of  $H$ , minus a third integer  $n_3$  times the valence energy of  $E(AO)$  (e.g.  $E(N) = -14.53414 \text{ eV}$ ) where the first integer can be 1, 2, 3..., and each of the second and third integers can be 0, 1, 2, 3....

61. The system of claim 60, wherein

$$E(\text{basis energies}) = n_1(-31.63536831 \text{ eV}) - n_2(-13.605804 \text{ eV}) - n_3 E(AO) \quad (15.40)$$

in the case that the MO bonds two atoms other than hydrogen,  $E(\text{basis energies})$  is  $n_1$  times the total energy of  $H_2$  where  $n_1$  is the number of equivalent bonds of the MO and the energy of  $H_2$ ,  $-31.63536831 \text{ eV}$ , Eq. (11.212) is the minimum energy possible for a prolate spheroidal MO:

$$E(\text{basis energies}) = n_1(-31.63536831 \text{ eV}) \quad (15.41)$$

$E_T(H_2MO)$ , is set equal to  $E(\text{basis energies})$ , and the semimajor axis  $a$  is solved.

62. The system of claims 23 or 60, wherein the semimajor axis  $a$  is solved from the equation of the form:

$$-\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] + E_T(AO/HO) = E(\text{basis energies}) \quad (15.42)$$

The distance from the origin of the  $H_2$ -type-ellipsoidal-MO to each focus  $c'$ , the internuclear distance  $2c'$ , and the length of the semiminor axis of the prolate spheroidal  $H_2$ -type MO  $b = c$  are solved from the semimajor axis  $a$  using Eqs. (15.2-15.4).

63. The system of claim 62, wherein the component energies are given by Eqs. (15.6-15.9) and (15.39).

64. The system of claim 57, wherein the total energy of the MO of the functional group,  $E_T(MO)$ , is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms and

$E_T(\text{atom} - \text{atom}, msp^3.AO)$ , the change in the energy of the AOs or HOs upon forming the bond.

65. The system of claim 64, wherein from Eqs. (15.39-15.40),  $E_T(MO)$  is

$$E_T(MO) = E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3.AO) \quad (15.43)$$

66. The system of claim 65, wherein during bond formation, the electrons undergo a reentrant oscillatory orbit with vibration of the nuclei, and the corresponding energy  $\bar{E}_{osc}$  is the sum of the Doppler,  $\bar{E}_D$ , and average vibrational kinetic energies,  $\bar{E}_{Kvib}$ :

$$\bar{E}_{osc} = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_{hv} \sqrt{\frac{2\bar{E}_K}{m_e c^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.44)$$

where  $n_1$  is the number of equivalent bonds of the MO,  $k$  is the spring constant of the equivalent harmonic oscillator, and  $\mu$  is the reduced mass.

67. The system of claim 66, wherein the angular frequency of the reentrant oscillation in the transition state corresponding to  $\bar{E}_D$  is determined by the force between the central field and the electrons in the transition state.

68. The system of claim 67, wherein the force and its derivative are given by

$$f(R) = -c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (15.45)$$

and

$$f'(a) = 2c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3} \quad (15.46)$$

such that the angular frequency of the oscillation in the transition state is given by

$$\omega = \sqrt{\frac{\left[ \frac{-3}{a} f(a) - f'(a) \right]}{m_e}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO} \frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 R^3}}{m_e}} \quad (15.47)$$

where  $R$  is the semimajor axis  $a$  or the semiminor axis  $b$  depending on the eccentricity of the bond that is most representative of the oscillation in the transition state,  $c_{BO}$  is the bond-

order factor which is 1 for a single bond and when the MO comprises  $n_1$  equivalent single bonds as in the case of functional groups,  $c_{BO}$  is 4 for an independent double bond as in the case of the  $CO_2$  and  $NO_2$  molecules and 9 for an independent triplet bond,  $C_{1o}$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of the oscillatory transition state of a chemical bond of the group, and  $C_{2o}$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond. Typically,  $C_{1o} = C_1$  and  $C_{2o} = C_2$ , the kinetic energy,  $E_K$ , corresponding to  $\bar{E}_D$  is given by Planck's equation for functional groups:

$$\bar{E}_K = \hbar\omega = \hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\epsilon_0 R^3}} \quad (15.48)$$

69. The system of claim 68, wherein the Doppler energy of the electrons of the reentrant orbit is

$$\bar{E}_D \cong E_{h\nu} \sqrt{\frac{2\bar{E}_K}{m_e c^2}} = E_{h\nu} \sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} \quad (15.49)$$

$\bar{E}_{osc}$  given by the sum of  $\bar{E}_D$  and  $\bar{E}_{Kvib}$  is

$$\bar{E}_{osc} (group) = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_{h\nu} \sqrt{\frac{2\hbar\sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\epsilon_0 R^3}}}{m_e c^2}} + E_{vib} \right) \quad (15.50)$$

$E_{h\nu}$  of a group having  $n_1$  bonds is given by  $E_T(MO)/n_1$  such that

$$\bar{E}_{osc} = n_1 (\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( E_T(MO)/n_1 \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.51)$$

$E_{T+osc} (Group)$  is given by the sum of  $E_T(MO)$  (Eq. (15.42)) and  $\bar{E}_{osc}$  (Eq. (15.51)):

$$\begin{aligned}
E_{T+osc} (Group) &= E_T (MO) + \bar{E}_{osc} \\
&= \left( \left[ \begin{aligned} & -\frac{n_1 e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1 C_2}}} \left[ c_1 c_2 \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1 C_2}}}{a - \sqrt{\frac{aa_0}{2C_1 C_2}}} - 1 \right] \right. \\ & \left. + E_T (AO / HO) + E_T (atom - atom, msp^3 .AO) \right] \\ & \left[ 1 + \sqrt{\frac{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}{\frac{m_e}{m_e c^2}}} \right] + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \end{aligned} \right] \\
&= \left( E(basis \text{ energies}) + E_T (atom - atom, msp^3 .AO) \right) \left[ 1 + \sqrt{\frac{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}{\frac{m_e}{m_e c^2}}} \right] + n_1 \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}}
\end{aligned}$$

(15.52).

70. The system of claim 69, wherein the total energy of the functional group  $E_T (group)$  is the sum of the total energy of the components comprising the energy contribution of the MO formed between the participating atoms,  $E(basis \text{ energies})$ , the change in the energy of the AOs or HOs upon forming the bond ( $E_T (atom - atom, msp^3 .AO)$ ), the energy of oscillation in the transition state, and the change in magnetic energy with bond formation,  $E_{mag}$ .

71. The system of claim 70, wherein from Eq. (15.52), the total energy of the group  $E_T (Group)$  is

$$\begin{aligned}
E_T (Group) &= \left( \begin{aligned} & \left( E(basis \text{ energies}) + E_T (atom - atom, msp^3 .AO) \right) \left[ 1 + \sqrt{\frac{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}{\frac{m_e}{m_e c^2}}} \right] \\ & + n_1 \bar{E}_{Kvib} + E_{mag} \end{aligned} \right)
\end{aligned}$$

(15.53).

72. The system of claim 71, wherein the change in magnetic energy  $E_{mag}$  which arises due to the formation of unpaired electrons in the corresponding fragments relative to the bonded group is given by

$$E_{mag} = c_3 \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r^3} = c_3 \frac{8\pi\mu_0 \mu_B^2}{r^3} \quad (15.54)$$

where  $r^3$  is the radius of the atom that reacts to form the bond and  $c_3$  is the number of electron pairs.

$$E_T (Group) = \left( E(basis \text{ energies}) + E_T (atom - atom, msp^3 .AO) \right) \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_0 \mu_B^2}{r^3} \quad (15.55).$$

73. The system of claim 72, wherein the total bond energy of the group  $E_D (Group)$  is the negative difference of the total energy of the group (Eq. (15.55)) and the total energy of the starting species given by the sum of  $c_4 E_{initial} (c_4 AO / HO)$  and  $c_5 E_{initial} (c_5 AO / HO)$ :

$$E_D (Group) = - \left( E(basis \text{ energies}) + E_T (atom - atom, msp^3 .AO) \right) \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}}}{m_e c^2}} \right] + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_0 \mu_B^2}{r_n^3} - (c_4 E_{initial} (AO / HO) + c_5 E_{initial} (c_5 AO / HO)) \quad (15.56).$$

74. The system of claim 70, wherein in the case of organic molecules, the atoms of the functional groups are energy matched to the  $C2sp^3$  HO such that

$$E(AO / HO) = -14.63489 \text{ eV} \quad (15.57)$$

70 For examples of  $E_{mag}$  from previous sections:

$$E_{mag}(C2sp^3) = c_3 \frac{8\pi\mu_o\mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o\mu_B^2}{(0.91771a_0)^3} = c_3 0.14803 \text{ eV} \quad (15.58)$$

$$E_{mag}(O2p) = c_3 \frac{8\pi\mu_o\mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o\mu_B^2}{a_0^3} = c_3 0.11441 \text{ eV} \quad (15.59)$$

$$E_{mag}(N2p) = c_3 \frac{8\pi\mu_o\mu_B^2}{r^3} = c_3 \frac{8\pi\mu_o\mu_B^2}{(0.93084a_0)^3} = c_3 0.14185 \text{ eV} \quad (15.60).$$

75. The system of claim 74, wherein in the general case of the solution of an organic functional group, the geometric bond parameters are solved from the semimajor axis and the relationships between the parameters by first using Eq. (15.42) to arrive at  $a$ , the remaining parameters are determined using Eqs. (15.1-15.5), the energies are given by Eqs. (15.52-15.59), and to meet the equipotential condition for the union of the  $H_2$ -type-ellipsoidal-MO and the HO or AO of the atom of a functional group, the factor  $c_2$  of a  $H_2$ -type ellipsoidal MO in principal Eqs. (15.42) and (15.52) may given by

(i) one:

$$c_2 = 1 \quad (15.61)$$

(ii) the ratio that is less than one of  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), and the magnitude of the Coulombic energy of the participating AO or HO of the atom,  $E_{Coulomb}(MO.atom,msp^3)$  given by Eqs. (15.19) and (15.31-15.32). For  $|E_{Coulomb}(MO.atom,msp^3)| > 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}} = \frac{13.605804 \text{ eV}}{|E_{Coulomb}(MO.atom,msp^3)|} \quad (15.62)$$

For  $|E_{Coulomb}(MO.atom,msp^3)| < 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ AorBsp}^3}}}{\frac{e^2}{8\pi\epsilon_0 a_0}} = \frac{|E_{Coulomb}(MO.atom,msp^3)|}{13.605804 \text{ eV}} \quad (15.63)$$

(iii) the ratio that is less than one of 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of H given by Eq. (1.243), and the magnitude of the valence energy,  $E(\text{valence})$ , of the participating AO or HO of the atom where  $E(\text{valence})$  is the ionization energy or  $E(\text{MO.atom}, msp^3)$  given by Eqs. (15.20) and (15.31-15.32). For  $|E(\text{valence})| > 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ or } Bsp^3}}} = \frac{13.605804 \text{ eV}}{|E(\text{valence})|} \quad (15.64)$$

For  $|E(\text{valence})| < 13.605804 \text{ eV}$ :

$$c_2 = \frac{\frac{e^2}{8\pi\epsilon_0 r_{A-B \text{ or } Bsp^3}}}{\frac{e^2}{8\pi\epsilon_0 a_0}} = \frac{|E(\text{valence})|}{13.605804 \text{ eV}} \quad (15.65)$$

(iv) the ratio that is less than one of the magnitude of the Coulombic energy of the participating AO or HO of a first atom,  $E_{\text{Coulomb}}(\text{MO.atom}, msp^3)$  given by Eqs. (15.19) and (15.31-15.32), and the magnitude of the valence energy,  $E(\text{valence})$ , of the participating AO or HO of a second atom to which the first is energy matched where  $E(\text{valence})$  is the ionization energy or  $E(\text{MO.atom}, msp^3)$  given by Eqs. (15.20) and (15.31-15.32). For  $|E_{\text{Coulomb}}(\text{MO.atom}, msp^3)| > E(\text{valence})$ :

$$c_2 = \frac{|E(\text{valence})|}{|E_{\text{Coulomb}}(\text{MO.atom}, msp^3)|} \quad (15.66)$$

For  $|E_{\text{Coulomb}}(\text{MO.atom}, msp^3)| < E(\text{valence})$ :

$$c_2 = \frac{|E_{\text{Coulomb}}(\text{MO.atom}, msp^3)|}{|E(\text{valence})|} \quad (15.67)$$

(v) the ratio that is less than one of the magnitude of the valence-level energies,  $E_n(\text{valence})$ , of the AO or HO of the nth participating atom of two that are energy matched



where  $E(\text{valence})$  is the ionization energy or  $E(\text{MO.atom}, msp^3)$  given by Eqs. (15.20) and (15.31-15.32):

$$c_2 = \frac{E_1(\text{valence})}{E_2(\text{valence})} \quad (15.68)$$

(vi) the factor that is the ratio of the hybridization factor  $c_2(1)$  of the valence AO or HO of a first atom and the hybridization factor  $c_2(2)$  of the valence AO or HO of a second atom to which the first is energy matched where  $c_2(n)$  is given by Eqs. (15.62-15.68); alternatively  $c_2$  is the hybridization factor  $c_2(1)$  of the valence AOs or HOs a first pair of atoms and the hybridization factor  $c_2(2)$  of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = \frac{c_2(1)}{c_2(2)} \quad (15.69)$$

(vii) the factor that is the product of the hybridization factor  $c_2(1)$  of the valence AO or HO of a first atom and the hybridization factor  $c_2(2)$  of the valence AO or HO of a second atom to which the first is energy matched where  $c_2(n)$  is given by Eqs. (15.62-15.69); alternatively  $c_2$  is the hybridization factor  $c_2(1)$  of the valence AOs or HOs a first pair of atoms and the hybridization factor  $c_2(2)$  of the valence AO or HO a third atom or second pair to which the first two are energy matched:

$$c_2 = c_2(1)c_2(2) \quad (15.70)$$

The hybridization factor  $c_2$  corresponds to the force constant  $k$  (Eqs. (11.65) and (13.58)). In the case that the valence or Coulombic energy of the AO or HO is less than 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), then  $C_2$  corresponding to  $k'$  (Eq. (15.1)) is given by Eqs. (15.62-15.70).

76. The system of claim 75, wherein specific examples of the factors  $c_2$  and  $C_2$  of a  $H_2$ -type ellipsoidal MO of Eq. (15.51) given in following sections are

$$c_2(C2sp^3HO \text{ to } F) = \frac{E(C, 2sp^3)}{E(F)} c_2(C2sp^3HO) = \frac{-14.63489 \text{ eV}}{-17.42282 \text{ eV}} (0.91771) = 0.77087;$$

$$c_2(C2sp^3HO \text{ to } Cl) = \frac{E(Cl)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-12.96764 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.81317;$$

$$c_2(C2sp^3HO \text{ to } Br) = \frac{E(Br)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-11.81381 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.74081;$$

$$c_2(C2sp^3HO \text{ to } I) = \frac{E(I)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-10.45126 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.65537;$$

$$c_2(C2sp^3HO \text{ to } O) = \frac{E(O)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-13.61806 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.85395;$$

$$c_2(H \text{ to } 1^\circ N) = \frac{E(N)}{E(C, 2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.35946 \text{ eV}} = 0.94627;$$

$$c_2(C2sp^3HO \text{ to } N) = \frac{E(N)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-14.53414 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.91140;$$

$$c_2(H \text{ to } 2^\circ N) = \frac{E(N)}{E(C, 2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.56407 \text{ eV}} = 0.93383;$$

$$C_2(S3p \text{ to } H) = \frac{E(S, 3p)}{E(H)} = \frac{-10.36001 \text{ eV}}{-13.60580 \text{ eV}} = 0.76144;$$

$$c_2(C2sp^3HO \text{ to } S) = \frac{E(S)}{E(C, 2sp^3)} c_2(C2sp^3HO) = \frac{-10.36001 \text{ eV}}{-14.63489 \text{ eV}} (0.91771) = 0.64965;$$

$$\begin{aligned} c_2(O \text{ to } S3sp^3 \text{ to } C2sp^3HO) &= \frac{E(O)}{E(S)} c_2(C2sp^3HO) \\ &= \frac{-13.61806 \text{ eV}}{-10.36001 \text{ eV}} (0.91771); \\ &= 1.20632 \end{aligned}$$

$$c_2(S3sp^3) = \frac{E_{Coulomb}(S3sp^3)}{E(H)} = \frac{-11.57099 \text{ eV}}{-13.60580 \text{ eV}} = 0.85045;$$

$$C_2(C2sp^3HO \text{ to } S3sp^3) = \frac{E(S3sp^3)}{E(C, 2sp^3)} c_2(S3sp^3) = \frac{-11.52126 \text{ eV}}{-14.63489 \text{ eV}} (0.85045) = 0.66951;$$

$$\begin{aligned}
 C_2(S3sp^3 \text{ to } O \text{ to } C2sp^3HO) &= \frac{E(S,3sp^3)}{E(O,2p)} c_2(C2sp^3HO) \\
 &= \frac{-11.52126 \text{ eV}}{-13.61806 \text{ eV}} (0.91771) ; \\
 &= 0.77641
 \end{aligned}$$

$$\begin{aligned}
 c_2(O \text{ to } N2p \text{ to } C2sp^3HO) &= \frac{E(O)}{E(N)} c_2(C2sp^3HO) \\
 &= \frac{-13.61806 \text{ eV}}{-14.53414 \text{ eV}} (0.91771); \\
 &= 0.85987
 \end{aligned}$$

$$c_2(N2p \text{ to } O2p) = \frac{c_2(C2sp^3HO \text{ to } N)}{c_2(C2sp^3HO \text{ to } O)} = \frac{0.91140}{0.85395} = 1.06727;$$

$$C_2(\text{benzene}C2sp^3HO) = c_2(\text{benzene}C2sp^3HO) = \frac{13.605804 \text{ eV}}{15.95955 \text{ eV}} = 0.85252;$$

$$\begin{aligned}
 c_2(\text{aryl}C2sp^3HO \text{ to } O) &= \frac{E(O)}{E(C,2sp^3)} c_2(\text{aryl}C2sp^3HO) \\
 &= \frac{-13.61806 \text{ eV}}{-14.63489 \text{ eV}} (0.85252) ; \\
 &= 0.79329
 \end{aligned}$$

$$c_2(H \text{ to anline } N) = \frac{E(N)}{E(C,2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.76868 \text{ eV}} = 0.92171,$$

$$\begin{aligned}
 c_2(\text{aryl}C2sp^3HO \text{ to } N) &= \frac{E(N)}{E(C,2sp^3)} c_2(\text{aryl}C2sp^3HO) \\
 &= \frac{-14.53414 \text{ eV}}{-14.63489 \text{ eV}} (0.85252) \\
 &= 0.84665
 \end{aligned}$$

$$c_2(H \text{ to anline } N) = \frac{E(N)}{E(C,2sp^3)} = \frac{-14.53414 \text{ eV}}{-15.76868 \text{ eV}} = 0.92171;$$

$$\begin{aligned}
 c_2(\text{aryl}C2sp^3HO \text{ to } N) &= \frac{E(N)}{E(C,2sp^3)} c_2(\text{aryl}C2sp^3HO) \\
 &= \frac{-14.53414 \text{ eV}}{-14.63489 \text{ eV}} (0.85252) , \\
 &= 0.84665
 \end{aligned}$$

and

$$C_2(S3p \text{ to aryl-type } C2sp^3HO) = \frac{E(S,3p)}{E(C,2sp^3)} = \frac{-10.36001 \text{ eV}}{-15.76868 \text{ eV}} = 0.65700.$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

77. The system of claim 1, wherein the parameters of the point of intersection of each  $H_2$ -type ellipsoidal MO and the  $A$ -atom AO are determined from the polar equation of the ellipse:

$$r = r_0 \frac{1+e}{1+e \cos \theta'} \quad (15.71).$$

78. The system of claim 77, wherein the radius of the  $A$  shell is  $r_A$ , and the polar radial coordinate of the ellipse and the radius of the  $A$  shell are equal at the point of intersection such that

$$r_A = (a - c') \frac{1 + \frac{c'}{a}}{1 + \frac{c'}{a} \cos \theta'} \quad (15.72).$$

79. The system of claim 78, wherein the polar angle  $\theta'$  at the intersection point is given by

$$\theta' = \cos^{-1} \left( \frac{a}{c'} \left( (a - c') \frac{1 + \frac{c'}{a}}{a_0} - 1 \right) \right) \quad (15.73).$$

80. The system of claim 79, wherein the angle  $\theta_{AAO}$  the radial vector of the  $A$  AO makes with the internuclear axis is

$$\theta_{AAO} = 180^\circ - \theta' \quad (15.74).$$

81. The system of claim 80, wherein the distance from the point of intersection of the orbitals to the internuclear axis is the same for both component orbitals such that the angle  $\omega t = \theta_{H_2MO}$  between the internuclear axis and the point of intersection of each  $H_2$ -type ellipsoidal MO with the  $A$  radial vector obeys the following relationship:

$$r_A \sin \theta_{AAO} = b \sin \theta_{H_2MO} \quad (15.75)$$

such that

$$\theta_{H_2MO} = \sin^{-1} \frac{r_a \sin \theta_{AAO}}{b} \quad (15.76).$$

82. The system of claim 81, wherein the distance  $d_{H_2MO}$  along the internuclear axis from the origin of  $H_2$ -type ellipsoidal MO to the point of intersection of the orbitals is given by

$$d_{H_2MO} = a \cos \theta_{H_2MO} \quad (15.77).$$

83. The system of claim 82, wherein the distance  $d_{AAO}$  along the internuclear axis from the origin of the  $A$  atom to the point of intersection of the orbitals is given by

$$d_{AAO} = c' - d_{H_2MO} \quad (15.78).$$

84. The system of claim 1, wherein in  $ACB$  MO comprising a linear combination of  $C-A$  bond and  $C-B$  bond MOs where  $C$  is the general central atom and a bond is possible between the  $A$  and  $B$  atoms of the  $C-A$  and  $C-B$  bonds, the  $\angle ACB$  bond angle is determined by the condition that the total energy of the  $H_2$ -type ellipsoidal MO between the terminal  $A$  and  $B$  atoms is zero.

85. The system of claim 84, wherein the force constant  $k'$  of a  $H_2$ -type ellipsoidal MO due to the equivalent of two point charges of at the foci is given by:

$$k' = \frac{C_1 C_2 2e^2}{4\pi\epsilon_0} \quad (15.79)$$

where  $C_1$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of a chemical bond of the specie which is 0.75 (Eq. (13.59)) for a terminal  $A-H$  ( $A$  is  $H$  or other atom) and 1 otherwise and  $C_2$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the chemical bond and is equal to the corresponding factor of Eqs. (15.42) and (15.52).

86. The system of claim 85, wherein the distance from the origin of the MO to each focus  $c'$  of the  $A-B$  ellipsoidal MO is given by:

$$c' = a \sqrt{\frac{\hbar^2 4\pi\epsilon_0}{m_e e^2 2C_1 C_2 a}} = \sqrt{\frac{aa_0}{2C_1 C_2}} \quad (15.80).$$

87. The system of claim 85, wherein the internuclear distance is

$$2c' = 2\sqrt{\frac{aa_0}{2C_1C_2}} \quad (15.81).$$

88. The system of claim 85, wherein the length of the semiminor axis of the prolate spheroidal  $A-B$  MO  $b=c$  is given by Eq. (15.4).

89. The system of claim 85, wherein the component energies and the total energy,  $E_T(H_2MO)$ , of the  $A-B$  bond are given by the energy equations (Eqs. (11.207-11.212), (11.213-11.217), and (11.239)) of  $H_2$  except that the terms based on charge are multiplied by  $c_{BO}$ , the bond-order factor which is 1 for a single bond and when the MO comprises  $n_1$  equivalent single bonds as in the case of functional groups.  $c_{BO}$  is 4 for an independent double bond as in the case of the  $CO_2$  and  $NO_2$  molecules.

90. The system of claim 85, wherein the kinetic energy term is multiplied by  $c'_{BO}$  which is 1 for a single bond, 2 for a double bond, and 9/2 for a triple bond, the electron energy terms are multiplied by  $c_1$ , the fraction of the  $H_2$ -type ellipsoidal MO basis function of a terminal chemical bond which is 0.75 (Eq. (13.233)) for a terminal  $A-H$  ( $A$  is  $H$  or other atom) and 1 otherwise.

91. The system of claim 85, wherein the electron energy terms are further multiplied by  $c'_2$ , the hybridization or energy-matching factor that results in an equipotential energy match of the participating at least two atomic orbitals of each terminal bond.

92. The system of claim 84, wherein when  $A-B$  comprises atoms other than  $H$ ,  $E_T(atom - atom, msp^3.AO)$ , the energy component due to the AO or HO's charge donation to the terminal MO, is added to the other energy terms to give  $E_T(H_2MO)$ :

$$E_T(H_2MO) = \frac{-e^2}{8\pi\epsilon_0 c'} \left[ c_1 c'_2 \left( 2c_{BO} - c'_{BO} \frac{a_0}{a} \right) \ln \frac{a+c'}{a-c'} - 1 \right] + E_T(atom - atom, msp^3.AO) \quad (15.82).$$

93. The system of claim 84, the radiation reaction force in the case of the vibration of  $A-B$  in the transition state corresponds to the Doppler energy,  $E_D$ , given by Eq. (11.181) that is dependent on the motion of the electrons and the nuclei.
94. The system of claim 93, wherein the total energy that includes the radiation reaction of the  $A-B$  MO is given by the sum of  $E_T(H_2MO)$  (Eq. (15.82)) and  $\bar{E}_{osc}$  given Eqs. (11.213-11.220), (11.231-11.236), and (11.239-11.240).
95. The system of claim 94, wherein the total energy  $E_T(A-B)$  of the  $A-B$  MO including the Doppler term is

$$E_T(A-B) = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 c'} \left[ c_1 c_2' \left( 2c_{BO} - c'_{BO} \frac{a_0}{a} \right) \ln \frac{a+c'}{a-c'} - 1 \right] + E_T(atom - atom, msp^3.AO) \right) \right] \\ \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_0 a^3}}}{m_e c^2}} + \frac{1}{2} \hbar \sqrt{\frac{c_{BO} \frac{c_1 c_2' e^2}{8\pi\epsilon_0 a^3} - \frac{c_{BO} e^2}{8\pi\epsilon_0 (a+c')^3}}{\mu}} \right] \quad (15.83)$$

where  $C_{1o}$  is the fraction of the  $H_2$ -type ellipsoidal MO basis function of the oscillatory transition state of the  $A-B$  bond which is 0.75 (Eq. (13.233)) in the case of  $H$  bonding to a central atom and 1 otherwise,  $C_{2o}$  is the factor that results in an equipotential energy match of the participating at least two atomic orbitals of the transition state of the chemical bond, and  $\mu = \frac{m_1 m_2}{m_1 + m_2}$  is the reduced mass of the nuclei given by Eq. (11.154).

96. The system of claim 95, wherein to match the boundary condition that the total energy of the  $A-B$  ellipsoidal MO is zero,  $E_T(A-B)$  given by Eq. (15.83) is set equal to zero and substitution of Eq. (15.81) into Eq. (15.83) gives

$$0 = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1C_2}}} \left[ c_1c'_2 \left( 2c_{BO} - c'_{BO} \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1C_2}}}{a - \sqrt{\frac{aa_0}{2C_1C_2}}} - 1 \right] + E_T \left( atom - atom, msp^3 . AO \right) \right) \right] \\ \left[ 1 + \sqrt{\frac{c_{BO} \frac{C_{10}C_{20}e^2}{4\pi\epsilon_0 a^3}}{m_e}} \right] + \frac{1}{2} \sqrt{\frac{c_{BO} \frac{c_1c'_2e^2}{8\pi\epsilon_0 a^3} - \frac{c_{BO}e^2}{8\pi\epsilon_0 \left( a + \sqrt{\frac{aa_0}{2C_1C_2}} \right)^3}}{\mu}} \right] \quad (15.84).$$

97. The system of claim 96, wherein the vibrational energy-term of Eq. (15.84) is determined by the forces between the central field and the electrons and those between the nuclei (Eqs. (11.141-11.145)).

98. The system of claim 96, wherein the electron-central-field force and its derivative are given by

$$f(a) = -c_{BO} \frac{c_1c'_2e^2}{4\pi\epsilon_0 a^3} \quad (15.85)$$

and

$$f'(a) = 2c_{BO} \frac{c_1c'_2e^2}{4\pi\epsilon_0 a^3} \quad (15.86).$$

99. The system of claim 97, wherein the nuclear repulsion force and its derivative are given by

$$f(a+c') = \frac{e^2}{8\pi\epsilon_0 (a+c')^2} \quad (15.87)$$

and

$$f'(a+c') = -\frac{e^2}{4\pi\epsilon_0 (a+c')^3} \quad (15.88)$$

such that the angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{\frac{-3}{a} f(a) - f'(a)}{\mu}} = \sqrt{\frac{k}{m_e}} = \sqrt{\frac{c_{BO} \frac{c_1c'_2e^2}{4\pi\epsilon_0 a^3} - \frac{e^2}{8\pi\epsilon_0 (a+c')^2}}{\mu}} \quad (15.89).$$



100. The system of claim 99, wherein since both terms of  $\bar{E}_{osc} = \bar{E}_D + \bar{E}_{Kvib}$  are small due to the large values of  $a$  and  $c'$ , an approximation of Eq. (15.84) which is evaluated to determine the bond angles of functional groups is given by

$$0 = \left[ \left( \frac{-e^2}{8\pi\epsilon_0 \sqrt{\frac{aa_0}{2C_1C_2}}} \left[ c_1 c_2' \left( 2 - \frac{a_0}{a} \right) \ln \frac{a + \sqrt{\frac{aa_0}{2C_1C_2}}}{a - \sqrt{\frac{aa_0}{2C_1C_2}}} - 1 \right] + E_T (atom - atom, msp^3 AO) \right) \right] \\ \left[ 1 + \sqrt{\frac{2\hbar \sqrt{\frac{c_1 e^2}{4\pi\epsilon_0 a^3}}}{m_e c^2}} + \frac{1}{2} \hbar \sqrt{\frac{\frac{c_1 e^2}{8\pi\epsilon_0 a^3} - \frac{e^2}{8\pi\epsilon_0 \left( a + \sqrt{\frac{aa_0}{2C_1C_2}} \right)^3}}{\mu}} \right] \quad (15.90).$$

101. The system of claim 100, wherein from the energy relationship given by Eq. (15.90) and the relationship between the axes given by Eqs. (15.2-15.5), the dimensions of the  $A-B$  MO can be solved.
102. The system of claim 101, wherein Eq. (15.90) is solved by the reiterative technique using a computer.
103. The system of claim 100, wherein a factor  $c_2$  of a given atom in the determination of  $c_2'$  for calculating the zero of the total  $A-B$  bond energy is given by Eqs. (15.62-15.65).
104. The system of claim 103, wherein in the case of a  $H-H$  terminal bond of an alkyl or alkenyl group,  $c_2'$  is the ratio of  $c_2$  of Eq. (15.62) for the  $H-H$  bond which is one and  $c_2$  of the carbon of the corresponding  $C-H$  bond:

$$c_2' = \frac{1}{c_2(C2sp^3)} = \frac{13.605804 \text{ eV}}{E_{Coulomb}(C-H \text{ } C2sp^3)} \quad (15.91)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

105. The system of claim 100, wherein in the case of the determination of the bond angle of the  $ACH$  MO comprising a linear combination of  $C-A$ -bond and  $C-H$ -bond MOs where  $A$  and  $C$  are general,  $C$  is the central atom, and  $c_2$  for an atom is given by Eqs. (15.62-15.70),  $c'_2$  of the  $A-H$  terminal bond is the ratio of  $c_2$  of the  $A$  atom for the  $A-H$  terminal bond and  $c_2$  of the  $C$  atom of the corresponding  $C-H$  bond:

$$c'_2 = \frac{c_2(A(A-H)msp^3)}{c_2(C(C-H)(msp^3))} \quad (15.92).$$

106. The system of claim 100, wherein in the case of the determination of the bond angle of the  $COH$  MO of an alcohol comprising a linear combination of  $C-O$ -bond and  $O-H$ -bond MOs where  $C$ ,  $O$ , and  $H$  are carbon, oxygen, and hydrogen, respectively,  $c'_2$  of the  $C-H$  terminal bond is 0.91771 since the oxygen and hydrogen atoms are at the Coulomb potential of a proton and an electron (Eqs. (1.236) and (10.162), respectively) that is energy matched to the  $C2sp^3$  HO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

107. The system of claim 100, wherein in the determination of the hybridization factor  $c'_2$  of Eq. (15.90) from Eqs. (15.62-15.70), the Coulombic energy,  $E_{Coulomb}(MO.atom,msp^3)$ , or the energy,  $E(MO.atom,msp^3)$ , the radius  $r_{A-B \text{ } A \text{ or } B sp^3}$  of the  $A$  or  $B$  AO or HO of the heteroatom of the  $A-B$  terminal bond MO such as the  $C2sp^3$  HO of a terminal  $C-C$  bond is calculated using Eq. (15.32) by considering  $\sum E_{r_{mol}}(MO,2sp^3)$ , the total energy donation to each bond with which it participates in bonding as it forms the terminal bond.

108. The system of claim 107, wherein the Coulombic energy  $E_{Coulomb}(MO.atom,msp^3)$  of the outer electron of the  $atom \text{ } msp^3$  shell is given by Eq. (15.19).

109. The system of claim 108, wherein in the case that during hybridization, at least one of the spin-paired AO electrons is unpaired in the hybridized orbital (HO), the energy change for the promotion to the unpaired state is the magnetic energy  $E(magnetic)$  (Eq. (15.15))

at the initial radius  $r$  of the AO electron, and the energy  $E(MO.atom,msp^3)$  of the outer electron of the  $atom\ msp^3$  shell is given by the sum of  $E_{Coulomb}(MO.atom,msp^3)$  and  $E(magnetic)$  (Eq. (15.20)).

110. The system of claim 99, wherein in the specific case of the terminal bonding of two carbon atoms, the  $c_2$  factor of each carbon given by Eq. (15.62) is determined using the Coulombic energy  $E_{Coulomb}(C-C\ C2sp^3)$  of the outer electron of the  $C2sp^3$  shell given by Eq. (15.19) with the radius  $r_{C-C\ C2sp^3}$  of each  $C2sp^3$  HO of the terminal  $C-C$  bond calculated using Eq. (15.32) by considering  $\sum E_{T_{mel}}(MO,2sp^3)$ , the total energy donation to each bond with which it participates in bonding as it forms the terminal bond including the contribution of the methylene energy,  $0.92918\ eV$  (Eq. (14.513)), corresponding to the terminal  $C-C$  bond. The corresponding  $E_T(atom-atom,msp^3.AO)$  in Eq. (15.90) is  $E_T(C-C\ C2sp^3) = -1.85836\ eV$ , wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

111. The system of claim 100, wherein in the case that the terminal atoms are carbon or other heteroatoms, the terminal bond comprises a linear combination of the HOs or AOs; thus,  $c'_2$  is the average of the hybridization factors of the participating atoms corresponding to the normalized linear sum:

$$c'_2 = \frac{1}{2}(c'_2(atom\ 1) + c'_2(atom\ 2)) \quad (15.93)$$

In the exemplary cases of  $C-C$ ,  $O-O$ , and  $N-N$  where  $C$  is carbon:

$$\begin{aligned} c'_2 &= \frac{1}{2} \left( \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-A_1 AO/HO}}} + \frac{\frac{e^2}{8\pi\epsilon_0 a_0}}{\frac{e^2}{8\pi\epsilon_0 r_{A-A_2 AO/HO}}} \right) \\ &= \frac{1}{2} \left( \frac{13.605804\ eV}{E_{Coulomb}(A-A_1 AO/HO)} + \frac{13.605804\ eV}{E_{Coulomb}(A-A_2 AO/HO)} \right) \end{aligned} \quad (15.94)$$

In the exemplary cases of  $C-N$ ,  $C-O$ , and  $C-S$ ,

$$c'_2 = \frac{1}{2} \left( \frac{13.605804 \text{ eV}}{E_{\text{Coulomb}}(C-B \text{ } C2sp^3)} + c_2(C \text{ to } B) \right) \quad (15.95)$$

where  $C$  is carbon and  $c_2(C \text{ to } B)$  is the hybridization factor of Eqs. (15.52) and (15.84) that matches the energy of the atom  $B$  to that of the atom  $C$  in the group.

112. The system of claim 97, wherein the corresponding  $E_T(\text{atom} - \text{atom}, msp^3.AO)$  term in Eq. (15.90) depends on the hybridization and bond order of the terminal atoms in the molecule, but typical values matching those used in the determination of the bond energies (Eq. (15.56)) are

$E_T(C-O \text{ } C2sp^3.O2p) = -1.44915 \text{ eV}$  ;  $E_T(C-O \text{ } C2sp^3.O2p) = -1.65376 \text{ eV}$  ;  
 $E_T(C-N \text{ } C2sp^3.N2p) = -1.44915 \text{ eV}$  ;  $E_T(C-S \text{ } C2sp^3.S2p) = -0.72457 \text{ eV}$  ;  
 $E_T(O-O \text{ } O2p.O2p) = -1.44915 \text{ eV}$  ;  $E_T(O-O \text{ } O2p.O2p) = -1.65376 \text{ eV}$  ;  
 $E_T(N-N \text{ } N2p.N2p) = -1.44915 \text{ eV}$  ;  $E_T(N-O \text{ } N2p.O2p) = -1.44915 \text{ eV}$  ;  
 $E_T(F-F \text{ } F2p.F2p) = -1.44915 \text{ eV}$  ;  $E_T(Cl-Cl \text{ } Cl3p.Cl3p) = -0.92918 \text{ eV}$  ;  
 $E_T(Br-Br \text{ } Br4p.Br4p) = -0.92918 \text{ eV}$  ;  $E_T(I-I \text{ } I5p.I5p) = -0.36229 \text{ eV}$  ;  
 $E_T(C-F \text{ } C2sp^3.F2p) = -1.85836 \text{ eV}$  ;  $E_T(C-Cl \text{ } C2sp^3.Cl3p) = -0.92918 \text{ eV}$  ;  
 $E_T(C-Br \text{ } C2sp^3.Br4p) = -0.72457 \text{ eV}$  ;  $E_T(C-I \text{ } C2sp^3.I5p) = -0.36228 \text{ eV}$  , and  
 $E_T(O-Cl \text{ } O2p.Cl3p) = -0.92918 \text{ eV}$  , wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to + 10%, if desired.

113. The system of claim 100, wherein in the case that the terminal bond is  $X-X$  where  $X$  is a halogen atom,  $c_1$  is one, and  $c'_2$  is the average (Eq. (15.93)) of the hybridization factors of the participating halogen atoms given by Eqs. (15.62-15.63) where

$E_{\text{Coulomb}}(MO.\text{atom}, msp^3)$  is determined using Eq. (15.32) and

$E_{\text{Coulomb}}(MO.\text{atom}, msp^3) = 13.605804 \text{ eV}$  for  $X = I$  .

114. The system of claim 113, wherein the factor  $C_1$  of Eq. (15.90) is one for all halogen atoms.

115. The system of claim 113, wherein the factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.
116. The system of claim 113, wherein for each of the halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $C_2$  is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with  $c_2(1)$  being that of the halogen given by Eq. (15.68) that matches the valence energy of  $X$  ( $E_1(\text{valence})$ ) to that of the  $C2sp^3$  HO ( $E_2(\text{valence}) = -14.63489 \text{ eV}$ , Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.
117. The system of claim 116, wherein  $E_T(\text{atom} - \text{atom}, msp^3.AO)$  of Eq. (15.90) is the maximum for the participating atoms which is  $-1.44915 \text{ eV}$ ,  $-0.92918 \text{ eV}$ ,  $-0.92918 \text{ eV}$ , and  $-0.33582 \text{ eV}$  for  $F$ ,  $Cl$ ,  $Br$ , and  $I$ , respectively, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.
118. The system of claim 100, wherein in the case that the terminal bond is  $C - X$  where  $C$  is a carbon atom and  $X$  is a halogen atom, the factors  $c_1$  and  $C_1$  of Eq. (15.90) are one for all halogen atoms.
119. The system of claim 118, wherein for  $X = F$ ,  $c'_2$  is the average (Eq. (15.95)) of the hybridization factors of the participating carbon and  $F$  atoms where  $c_2$  for carbon is given by Eq. (15.62) and  $c_2$  for fluorine matched to carbon is given by Eq. (15.70) with  $c_2(1)$  for the fluorine atom given by Eq. (15.68) that matches the valence energy of  $F$  ( $E_1(\text{valence}) = -17.42282 \text{ eV}$ ) to that of the  $C2sp^3$  HO ( $E_2(\text{valence}) = -14.63489 \text{ eV}$ ,

Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

120. The system of claim 119, wherein the factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that  $13.605804 \text{ eV}$ , the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

121. The system of claim 119, wherein for each of the other halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $c'_2$  is the hybridization factor of the participating carbon atom since the halogen atom is energy matched to the carbon atom.

122. The system of claim 121, wherein the  $C_2$  of the terminal-atom bond matches that used to determine the energies of the corresponding  $C - X$  -bond MO.

123. The system of claim 122, wherein  $C_2$  is the hybridization factor of Eq. (15.52) given by Eq. (15.70) with  $c_2(1)$  for the halogen atom given by Eq. (15.68) that matches the valence energy of  $X$  ( $E_1(\text{valence})$ ) to that of the  $C2sp^3$  HO ( $E_2(\text{valence}) = -14.63489 \text{ eV}$ , Eq. (15.25)) and to the hybridization of  $C2sp^3$  HO ( $c_2(2) = 0.91771$ , Eq. (13.430)), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

124. The system of claim 123, wherein  $E_T(\text{atom} - \text{atom}, msp^3.AO)$  of Eq. (15.90) is the maximum for the participating atoms which is  $-1.85836 \text{ eV}$ ,  $-0.92918 \text{ eV}$ ,  $-0.72457 \text{ eV}$ , and  $-0.33582 \text{ eV}$  for  $F$ ,  $Cl$ ,  $Br$ , and  $I$ , respectively, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

125. The system of claim 119, wherein in the case that the terminal bond is  $H-X$  corresponding to the angle of the atoms  $H-C-X$  where  $C$  is a carbon atom and  $X$  is a halogen atom, the factors  $c_1$  and  $C_1$  of Eq. (15.90) are 0.75 for all halogen atoms.
126. The system of claim 119, wherein for  $X = F$ ,  $c'_2$  is given by Eq. (15.69) with  $c_2$  of the participating carbon and  $F$  atoms given by Eq. (15.62) and Eq. (15.65), respectively.
127. The system of claim 126, wherein the factor  $C_2$  of fluorine is one since it is the only halogen wherein the ionization energy is greater than that 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of  $H$  given by Eq. (1.243), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.
128. The system of claim 127, wherein for each of the other halogens,  $Cl$ ,  $Br$ , and  $I$ ,  $c'_2$  is also given by Eq. (15.69) with  $c_2$  of the participating carbon given by Eq. (15.62) and  $c_2$  of the participating  $X$  atom given by  $c_2 = 0.91771$  (Eq. (13.430)) since the  $X$  atom is energy matched to the  $C2sp^3$  HO.
129. The system of claim 128, wherein  $C_2$  is given by Eq. (15.65) for the corresponding atom  $X$  where  $C_2$  matches the energy of the atom  $X$  to that of  $H$ .
130. The system of claim 100, wherein the distance between the two atoms  $A$  and  $B$  of the general molecular group  $ACB$  when the total energy of the corresponding  $A-B$  MO is zero, the corresponding bond angle can be determined from the law of cosines:  

$$s_1^2 + s_2^2 - 2s_1s_2\cos\theta = s_3^2 \quad (15.96).$$
131. The system of claim 130, wherein with  $s_1 = 2c'_{C-A}$ , the internuclear distance of the  $C-A$  bond,  $s_2 = 2c'_{C-B}$ , the internuclear distance of each  $C-B$  bond, and  $s_3 = 2c'_{A-B}$ , the internuclear distance of the two terminal atoms, the bond angle  $\theta_{\angle ACB}$  between the  $C-A$  and  $C-B$  bonds is given by

$$(2c'_{C-A})^2 + (2c'_{C-B})^2 - 2(2c'_{C-A})(2c'_{C-B})\cos\theta = (2c'_{A-B})^2 \quad (15.97)$$

$$\theta_{\angle ACB} = \cos^{-1} \left( \frac{(2c'_{C-A})^2 + (2c'_{C-B})^2 - (2c'_{A-B})^2}{2(2c'_{C-A})(2c'_{C-B})} \right) \quad (15.98).$$

132. The system of claim 131, wherein the structure  $C_b C_a (O_a) O_b$  wherein  $C_a$  is bound to  $C_b$ ,  $O_a$ , and  $O_b$ , the three bonds are coplanar and two of the angles are known, say  $\theta_1$  and  $\theta_2$ , then the third  $\theta_3$  can be determined geometrically:

$$\theta_3 = 360 - \theta_1 - \theta_2 \quad (15.99)$$

133. The system of claim 131, wherein in the general case that two of the three coplanar bonds are equivalent and one of the angles is known, say  $\theta_1$ , then the second and third can be determined geometrically:

$$\theta_2 = \theta_3 = \frac{(360 - \theta_1)}{2} \quad (15.100).$$

134. The system of claim 1, wherein in the general case where the group comprises three  $A-B$  bonds having  $B$  as the central atom at the apex of a pyramidal structure formed by the three bonds with the  $A$  atoms at the base in the xy-plane.

135. The system of claim 134, wherein the  $C_{3v}$  axis centered on  $B$  is defined as the vertical or z-axis, and any two  $A-B$  bonds form an isosceles triangle, and the angle of the bonds and the distances from and along the z-axis are determined from the geometrical relationships given by Eqs. (13.412-13.416):

the distance  $d_{origin-B}$  from the origin to the nucleus of a terminal  $B$  atom is given by

$$d_{origin-B} = \frac{2c'_{B-B}}{2 \sin 60^\circ} \quad (15.101)$$

the height along the z-axis from the origin to the  $A$  nucleus  $d_{height}$  is given by

$$d_{height} = \sqrt{(2c'_{A-B})^2 - (d_{origin-B})^2}, \text{ and } (15.102)$$

the angle  $\theta_v$  of each  $A-B$  bond from the z-axis is given by



$$\theta_v = \tan^{-1} \left( \frac{d_{origin-B}}{d_{height}} \right) \quad (15.103).$$

136. The system of claim 135, wherein in the case where the central atom  $B$  is further bound to a fourth atom  $C$  and the  $B-C$  bond is along the  $z$ -axis. Then, the bond  $\theta_{\angle ABC}$  given by Eq. (14.206) is

$$\theta_{\angle ABC} = 180 - \theta_v. \quad (15.104).$$

137. The system of claim 134, wherein in the plane defined by a general  $ACA$  MO comprising a linear combination of two  $C-A$ -bond MOs where  $C$  is the central atom, the dihedral angle  $\theta_{\angle BC/ACA}$  between the  $ACA$ -plane and a line defined by a third bond with  $C$ , specifically that corresponding to a  $C-B$ -bond MO, is calculated from the bond angle  $\theta_{\angle ACA}$  and the distances between the  $A$ ,  $B$ , and  $C$  atoms.

138. The system of claim 137, wherein the distance  $d_1$  along the bisector of  $\theta_{\angle ACA}$  from  $C$  to the internuclear-distance line between  $A$  and  $A$ ,  $2c'_{A-A}$ , is given by

$$d_1 = 2c'_{C-A} \cos \frac{\theta_{\angle ACA}}{2} \quad (15.105)$$

where  $2c'_{C-A}$  is the internuclear distance between  $A$  and  $C$ .

139. The system of claim 138, wherein the atoms  $A$ ,  $A$ , and  $B$  define the base of a pyramid.

140. The system of claim 139, wherein the pyramidal angle  $\theta_{\angle ABA}$  can be solved from the internuclear distances between  $A$  and  $A$ ,  $2c'_{A-A}$ , and between  $A$  and  $B$ ,  $2c'_{A-B}$ , using the law of cosines (Eq. (15.98)):

$$\theta_{\angle ABA} = \cos^{-1} \left( \frac{(2c'_{A-B})^2 + (2c'_{A-B})^2 - (2c'_{A-A})^2}{2(2c'_{A-B})(2c'_{A-B})} \right) \quad (15.106).$$

141. The system of claim 140, wherein the distance  $d_2$  along the bisector of  $\theta_{\angle ABA}$  from  $B$  to the internuclear-distance line  $2c'_{A-A}$ , is given by

$$d_2 = 2c'_{A-B} \cos \frac{\theta_{\angle ABA}}{2} \quad (15.107).$$

142. The system of claim 141, wherein the lengths  $d_1$ ,  $d_2$ , and  $2c'_{C-B}$  define a triangle wherein the angle between  $d_1$  and the internuclear distance between  $B$  and  $C$ ,  $2c'_{C-B}$ , is the dihedral angle  $\theta_{\angle BC/ACA}$  that can be solved using the law of cosines (Eq. (15.98)):

$$\theta_{\angle BC/ACA} = \cos^{-1} \left( \frac{d_1^2 + (2c'_{C-B})^2 - d_2^2}{2d_1(2c'_{B-C})} \right) \quad (15.108).$$

143. The system of claim 1, wherein the specie are solved using the solutions of organic chemical functional groups as basis elements wherein the structures and energies where linearly added to achieve the molecular solutions, each functional group can be treated as a building block to form any desired molecular solution from the corresponding linear combination, each functional group element was solved using the atomic orbital and hybrid orbital spherical orbitalsphere solutions bridged by molecular orbitals comprised of the  $H_2$ -type prolate spheroidal solution given in the Nature of the Chemical Bond of Hydrogen-Type Molecules section, the energy of each MO was matched at the HO or AO by matching the hybridization and total energy of the MO to the AOs and HOs, the energy  $E_{mag}$  (e.g. given by Eq. (15.58)) for a  $C2sp^3$  HO and Eq.(15.59) for an  $O2p$  AO) was subtracted for each set of unpaired electrons created by bond breakage.

144. They system of claim 143, wherein the bond energy is not equal to the component energy of each bond as it exists in the specie, although, they are close.

145. The system of claim 143, wherein the total energy of each group is its contribution to the total energy of the specie as a whole.

146. The system of claim 143, wherein the determination of the bond energies for the creation of the separate parts must take into account the energy of the formation of any

radicals and any redistribution of charge density within the pieces and the corresponding energy change with bond cleavage.

147. The system of claim 143, wherein the vibrational energy in the transition state is dependent on the other groups that are bound to a given functional group, which will effect the functional-group energy, however because the variations in the energy based on the balance of the molecular composition are typically of the order of a few hundreds of electron volts at most, they are neglected.
148. The system of claim 143, wherein the energy of each functional-group MO bonding to a given carbon HO is independently matched to the HO by subtracting the contribution to the change in the energy of the HO from the total MO energy given by the sum of the MO contributions and  $E(C, 2sp^3) = -14.63489 \text{ eV}$  (Eq. (13.428)).
149. The system of claim 143, wherein the intercept angles are determined from Eqs. (15.71-15.78) using the final radius of the HO of each atom.
150. The system of claim 143, wherein a final carbon-atom radius is determined using Eqs. (15.32) wherein the sum of the energy contributions of each atom to all the MOs in which it participates in bonding is determined.
151. The system of claim 150, wherein the final radius is used in Eqs. (15.19) and (15.20) to calculate the final valence energy of the HO of each atom at the corresponding final radius.
152. The system of claim 151, wherein the radius of any bonding heteroatom that contributes to a MO is calculated in the same manner, and the energy of its outermost shell is matched to that of the MO by the hybridization factor between the carbon-HO energy and the energy of the heteroatomic shell.
153. The system of claim 150, wherein the donation of electron density to the AOs and HOs reduces the energy.

154. The system of claim 143, wherein the donation of the electron density to the MO's at each AO or HO is that which causes the resulting energy to be divided equally between the participating AOs or HOs to achieve energy matching.
155. The system of claim 1, wherein the molecular solutions are used to design synthetic pathways and predict product yields based on equilibrium constants calculated from the heats of formation.
156. The system of claim 1, wherein the new stable compositions of matter are predicted as well as the structures of combinatorial chemistry reactions.
157. The system of claim 1, wherein pharmaceutical applications include the ability to graphically or computationally render the structures of drugs that permit the identification of the biologically active parts of the specie to be identified from the common spatial charge-density functions of a series of active species.
158. The system of claim 1, wherein novel drugs are designed according to geometrical parameters and bonding interactions with the data of the structure of the active site of the drug.
159. The system of claim 1, wherein to calculate conformations, folding, and physical properties, the exact solutions of the charge distributions in any given specie are used to calculate the fields, and from the fields, the interactions between groups of the same specie or between groups on different species are calculated wherein the interactions are distance and relative orientation dependent.
160. The system of claim 159, the fields and interactions can be determined using a finite-element-analysis approach of Maxwell's equations.
161. The system of claim 1, wherein in the case where three sets of  $C = C$ -bond MOs form bonds between the two carbon atoms of each molecule to form a six-member ring such that the six resulting bonds comprise eighteen paired electrons, and each bond

comprises a linear combination of two MOs wherein each comprises two  $C2sp^3$  HOs and 75% of a  $H_2$ -type ellipsoidal MO divided between the  $C2sp^3$  HOs:

$$\left( \begin{array}{l} 3(2 C2sp^3 + 0.75 H_2 MO) \rightarrow 3(C=C)^{4e} - \text{ethylene-type-bond MO} \\ \rightarrow 6(C=C)^{3e} - \text{bond MO of benzene} \end{array} \right) \quad (15.142).$$

162. The system of claim 162, wherein the linear combination of each  $H_2$ -type ellipsoidal MO with each  $C2sp^3$  HO further comprises an excess 25% charge-density contribution per bond from each  $C2sp^3$  HO to the  $C=C$ -bond MO to achieve an energy minimum.

163. The system of claim 163, wherein the dimensional parameters of each bond  $C=C$ -bond are determined using Eqs. (15.42) and (15.1-15.5) in a form that are the same equations as those used to determine the same parameters of the  $C=C$ -bond MO of ethylene (Eqs. (14.242-14.268)) while matching the boundary conditions of the structure of benzene.

164. The system of claim 161, wherein hybridization with 25% electron donation to each  $C=C$ -bond gives rise to the  $C_{benzene} 2sp^3$  HO-shell Coulombic energy  $E_{Coulomb}(C_{benzene}, 2sp^3)$  given by Eq. (14.245).

165. The system of claim 161, wherein to meet the equipotential condition of the union of the six  $C2sp^3$  HOs,  $c_2$  and  $C_2$  of Eq. (15.42) for the aromatic  $C=C$ -bond MO is given by Eq. (15.62) as the ratio of 15.95955 eV, the magnitude of  $E_{Coulomb}(C_{benzene}, 2sp^3)$  (Eq. (14.245)), and 13.605804 eV, the magnitude of the Coulombic energy between the electron and proton of  $H$  (Eq. (1.243)):

$$C_2(benzeneC2sp^3 HO) = c_2(benzeneC2sp^3 HO) = \frac{13.605804 \text{ eV}}{15.95955 \text{ eV}} = 0.85252 \quad (15.143)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

166. The system of claim 161, wherein the energies of each  $C=C$ <sup>3e</sup> bond of benzene are determined using the same equations as those of ethylene (Eqs. (14.251-14.253) and (14.319-14.333) with the parameters of benzene.

167. The system of claim 161, wherein ethylene serves as a basis element for the  $C=C$ <sup>3e</sup> bonding of benzene wherein each of the six  $C=C$ <sup>3e</sup> bonds of benzene comprises  $(0.75)(4) = 3$  electrons according to Eq. (15.142).

168. The system of claim 161, wherein the total energy of the bonds of the eighteen electrons of the  $C=C$ <sup>3e</sup> bonds of benzene,  $E_T(C_6H_6, C=C)^{3e}$ , is given by  $(6)(0.75)$  times  $E_{T+osc}(C=C)$  (Eq. (14.492)), the total energy of the  $C=C$ <sup>3e</sup>-bond MO of benzene including the Doppler term, minus eighteen times  $E(C, 2sp^3)$  (Eq. (14.146)), the initial energy of each  $C2sp^3$  HO of each  $C$  that forms the  $C=C$ <sup>3e</sup> bonds of bond order two.

169. The system of claim 161, wherein the total energy of the six  $C=C$ <sup>3e</sup> bonds of benzene with three electron per aromatic bond given by Eq. (14.493) is

$$\begin{aligned} E_T(C_6H_6, C=C)^{3e} &= (6)(0.75)E_{T+osc}(C=C) - (6)(3)E(C, 2sp^3) \\ &= (6)(0.75)(-66.05796 \text{ eV}) - 18(-14.63489 \text{ eV}) \quad (15.144) \\ &= -297.26081 \text{ eV} - (-263.42798 \text{ eV}) \\ &= -33.83284 \text{ eV} \end{aligned}$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

170. The system of claim 161, wherein the results of benzene can be generalized to the class of aromatic and heterocyclic compounds.  $E_{hv}$  of an aromatic bond is given by

$E_T(H_2)$  (Eqs. (11.212) and (14.486)), the maximum total energy of each  $H_2$ -type MO such that

$$\bar{E}_{osc} = n_1(\bar{E}_D + \bar{E}_{Kvib}) = n_1 \left( -31.63536831 \text{ eV} \sqrt{\frac{2\bar{E}_K}{Mc^2}} + \frac{1}{2} \hbar \sqrt{\frac{k}{\mu}} \right) \quad (15.145),$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

171. The system of claim 170, wherein the factor of 0.75 corresponding to the three electrons per aromatic bond of bond order two given in the Benzene Molecule ( $C_6H_6$ ) section modifies Eqs. (15.52-15.56).

172. The system of claim 171, wherein the multiplication of the total energy given by Eq. (15.55) by  $f_1 = 0.75$  with the substitution of Eq. (15.145) gives the total energy of the aromatic bond:

$$E_T(\text{Group}) = f_1 \left( \begin{array}{l} E(\text{basis energies}) + E_T(\text{atom-atom,msp}^3.AO) \\ -31.63536831 \text{ eV} \sqrt{\frac{2\hbar \sqrt{\frac{C_{1o}C_{2o}e^2}{4\pi\epsilon_o R^3}}}{m_e} + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o\mu_B^2}{r^3}} \end{array} \right) \quad (15.146)$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

173. The system of claim 161, wherein the total bond energy of the aromatic group  $E_D(\text{Group})$  is the negative difference of the total energy of the group (Eq. (15.146)) and the total energy of the starting species given by the sum of  $c_4 E_{initial}(c_4 AO / HO)$  and  $c_5 E_{initial}(c_5 AO / HO)$ :

$$E_D(\text{Group}) = - \left[ f_1 \left( \begin{aligned} &E(\text{basis energies}) + E_T(\text{atom} - \text{atom}, msp^3, AO) \\ &- 31.63536831 \text{ eV} \sqrt{\frac{C_{1o} C_{2o} e^2}{4\pi\epsilon_o R^3}} \frac{2\hbar}{m_e c^2} + n_1 \bar{E}_{Kvib} + c_3 \frac{8\pi\mu_o \mu_B^2}{r^3} \end{aligned} \right) - (c_4 E_{initial}(AO / HO) + c_5 E_{initial}(c_5 AO / HO)) \right]$$

(15.147), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

174. The system of claim 161, wherein benzene is considered as comprising chemical bonds between six *CH* radicals wherein each radical comprises a chemical bond between carbon and hydrogen atoms, energy components of  $V_e$ ,  $V_p$ ,  $T$ ,  $V_m$ , and  $E_T$  are the same as those of the hydrogen carbide radical, except that  $E_T(C = C, 2sp^3) = -1.13379 \text{ eV}$  (Eq. (14.247)) is subtracted from  $E_T(CH)$  of Eq. (13.495) to match the energy of each *C-H*-bond MO to the decrease in the energy of the corresponding  $C2sp^3$  HO, wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

175. The system of claim 174, wherein in the corresponding generalization of the aromatic *CH* group, the geometrical parameters are determined using Eq. (15.42) and Eqs. (15.1-15.5) with  $E_T(\text{atom} - \text{atom}, msp^3, AO) = -1.13379 \text{ eV}$  wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

176. The system of claim 174, wherein the total energy of the benzene *C-H*-bond MO,  $E_{T_{benzene}}(C-H)$ , given by Eq. (14.467) is the sum of  $0.5E_T(C = C, 2sp^3)$ , the energy change of each  $C2sp^3$  shell per single bond due to the decrease in radius with the formation of the corresponding  $C=C$ -bond MO (Eq. (14.247)), and  $E_{T_{benzene}}(CH)$ , the  $\sigma$  MO contribution given by Eq. (14.441). In the corresponding generalization of the



aromatic  $CH$  group, the energy parameters are determined using Eqs. (15.146-15.147)

with  $f_1 = 1$  and  $E_T(atom - atom, msp^3.AO) = \frac{-1.13379 \text{ eV}}{2}$ , wherein the calculated and

measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

177. The system of claim 176, wherein the energy contribution to the single aromatic  $CH$  bond is one half that of the  $C=C^{3e}$  double bond contribution, which matches the energies of the  $CH$  and  $C=C^{3e}$  aromatic groups, conserves the electron number with the equivalent charge density as that of  $s = 1$  in Eqs. (15.18-15.21), and further gives a minimum energy for the molecule.

178. The system of claim 177, wherein the breakage of the aromatic  $C=C^{3e}$  bonds to give  $CH$  groups creates unpaired electrons in these fragments that corresponds to  $c_3 = 1$  in Eq. (15.56) with  $E_{mag}$  given by Eq. (15.58).

179. The system of claim 178, wherein each of the  $C-H$  bonds of benzene comprises two electrons according to Eq. (14.439).

180. The system of claim 179, wherein from the energy of each  $C-H$  bond,  $-E_{D_{benzene}}(^{12}CH)$  (Eq. (14.477)), the total energy of the twelve electrons of the six  $C-H$  bonds of benzene,  $E_T(C_6H_6, C-H)$ , given by Eq. (14.494) is

$$E_T(C_6H_6, C-H) = (6) \left( -E_{D_{benzene}}(^{12}CH) \right) = 6(-3.90454 \text{ eV}) = -23.42724 \text{ eV}$$

(15.148), wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

181. The system of claim 174, wherein the total bond dissociation energy of benzene,

$E_D(C_6H_6)$ , given by Eq. (14.495) is the negative sum of  $E_T\left(C_6H_6, C=C^{3e}\right)$  (Eq.

(14.493)) and  $E_T(C_6H_6, C-H)$  (Eq. (14.494)):

$$\begin{aligned}
 E_D(C_6H_6) &= -\left( E_T\left( C_6H_6, C \equiv C^{3e} \right) + E_T\left( C_6H_6, C-H \right) \right) \\
 &= -\left( (-33.83284 \text{ eV}) + (-23.42724 \text{ eV}) \right) \quad (15.149) \\
 &= 57.2601 \text{ eV}
 \end{aligned}$$

wherein the calculated and measured values and constants recited in the equations herein can be adjusted, for example, up to  $\pm 10\%$ , if desired.

182. The system of claim 181, wherein using the parameters given in Tables 15.214 and 15.216 in the general equations (Eqs. (15.42), (15.1-15.5), and (15.146-15.147)) reproduces the results for benzene given in the Benzene Molecule ( $C_6H_6$ ) section as shown in Tables 15.214 and 15.216.
183. A system of computing and rendering the nature of at least one specie selected from a group of diatomic molecules having at least one atom that is other than hydrogen, polyatomic molecules, molecular ions, polyatomic molecular ions, or molecular radicals, or any functional group therein, comprising physical, Maxwellian solutions of charge, mass, and current density functions of said specie, said system comprising:
- processing means for processing physical, Maxwellian equations representing charge, mass, and current density functions of said specie to produce at least one Maxwellian solution; and
  - an output means for outputting the Maxwellian solution.
184. The system of claim 183, further comprising a data transfer system for inputting numerical data into or out of a computational components and storage components of the main system.
185. The system of claim 183, further comprising a spreadsheet containing solutions of the bond parameters with output in a standard spreadsheet format.
186. The system of claim 185, further comprising a data-handling program to transfer data from the spreadsheets into the main program.

187. The system of claim 183, wherein output may be at least one of graphical, simulation, text, and numerical data.
188. The system of claim 187, wherein the output may be the calculation of at least one of: (1) a bond distance between two of the atoms; (2) a bond angle between three of the atoms; (3) a bond energy between two of the atoms; (4) orbital intercept distances and angles; and (5) charge-density functions of atomic, hybridized, and molecular orbitals, wherein the bond distance, bond angle, and bond energy are calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration
189. The system of claim 183, wherein the charge, current, energy, and geometrical parameters are output to be inputs to other programs that can be used in further applications.
190. The system of claim 189, wherein the data of heats of formation can be input to another program to be used to predict stability (existence of compounds) equilibrium constants and to predict synthetic pathways.
191. The system of claim 190, wherein novel composition of matters can be discovered by calculating at least one of a bond distance between two of the atoms, a bond angle between three of the atoms, and a bond energy between two of the atoms, orbital intercept distances and angles, charge-density functions of atomic, hybridized, and molecular orbitals, the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.
192. The system of claim 190, wherein the charge and current density functions can be used to predict the electric and magnetic fields of the species to determine other properties due to the interaction of the fields between species.

193. The system of claim 192, wherein finite-element analysis is used to predict or calculate the interaction and resulting properties, such as the freezing point, boiling point, density, viscosity, and refractive index.
194. The system of claim 183, wherein the output data can be used to give thermodynamic, spectroscopic, and other properties, aid in drug design and other applications with or without direct visualization.
195. The system of claim 183, wherein the data can be input into other programs of the system, which calculate thermodynamic and other properties, or performs a simulation, such as a chemical reaction or molecular dynamics.
196. A method of using any of the systems of claims 1-195.
197. A use of any system of claims 1-195.
198. A composition of matter comprising a plurality of atoms, the improvement comprising a novel property or use discovered by calculation of at least one of  
a bond distance between two of the atoms,  
a bond angle between three of the atoms, and  
a bond energy between two of the atoms,  
orbital intercept distances and angles,  
charge-density functions of atomic, hybridized, and molecular orbitals,  
the bond distance, bond angle, and bond energy being calculated from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate under acceleration.
199. A composition of matter according to claim 198, wherein the novel property is a new pharmaceutical use.
200. A composition of matter according to claim 198 that is novel, wherein the novel property is stability at room temperature of a new arrangement of atoms or ions.

201. A novel composition of matter discovered by calculating at least one of  
a bond distance between two of the atoms,  
a bond angle between three of the atoms, and  
a bond energy between two of the atoms,  
orbital intercept distances and angles,  
charge-density functions of atomic, hybridized, and molecular orbitals,  
the bond distance, bond angle, and bond energy being calculated from physical solutions of  
the charge, mass, and current density functions of atoms and atomic ions, which solutions are  
derived from Maxwell's equations using a constraint that a bound electron(s) does not radiate  
under acceleration.

202. A system of determining at least one of  
a bond distance between two of the atoms,  
a bond angle between three of the atoms, and  
a bond energy between two of the atoms,  
orbital intercept distances and angles,  
charge-density functions of atomic, hybridized, and molecular orbitals,  
wherein the bond distance, bond angle, and bond energy being calculated from physical  
solutions of the charge, mass, and current density functions of atoms and atomic ions, which  
solutions are derived from Maxwell's equations using a constraint that the bound electron(s)  
does not radiate under acceleration.

203. The system of claim 202, further comprising discovering a new composition of  
matter.

204. A system of claim 1-195, wherein the calculated and measured values and constants  
recited therein can be adjusted up to  $\pm 10\%$  as desired.

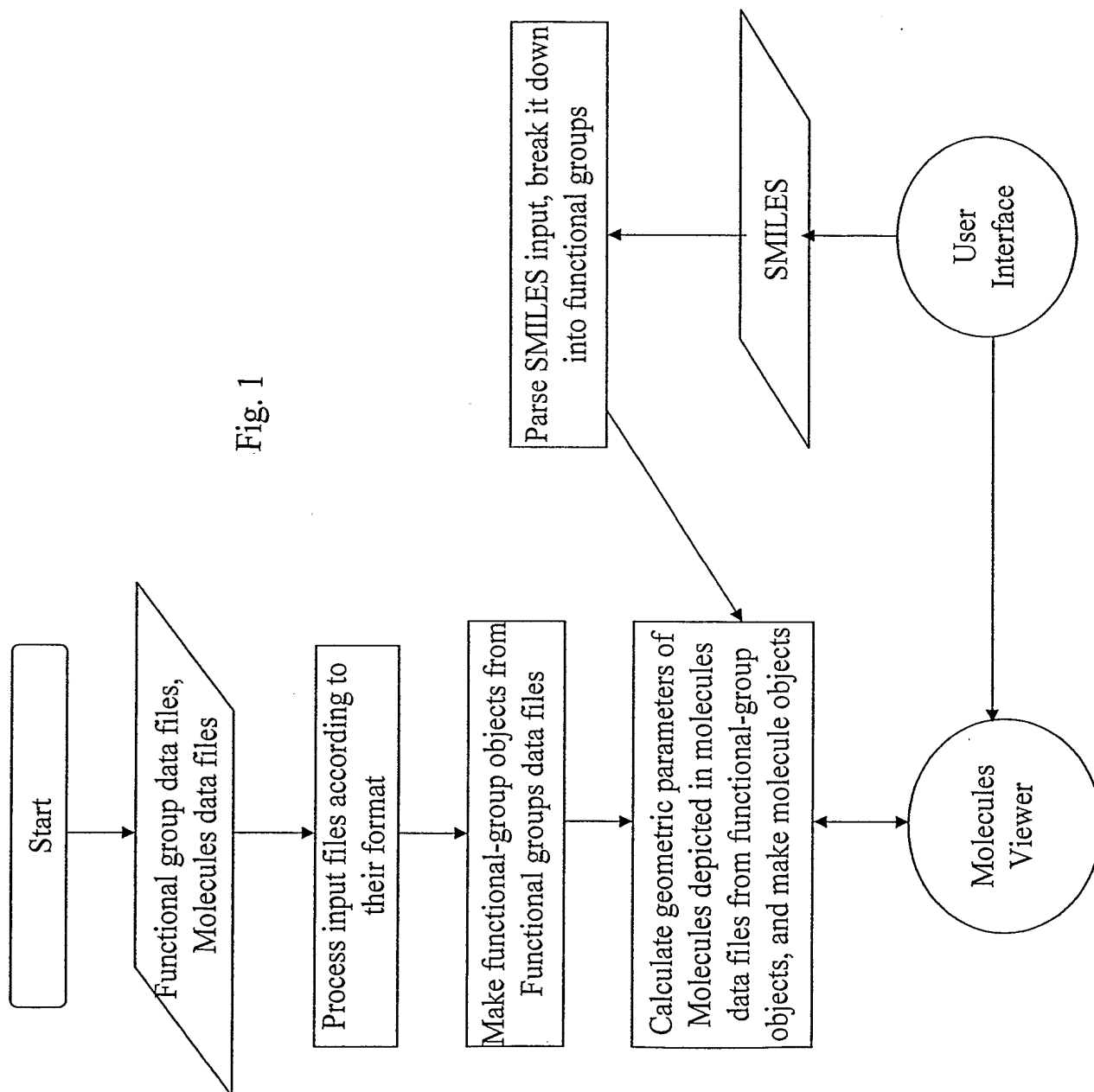


Fig. 2

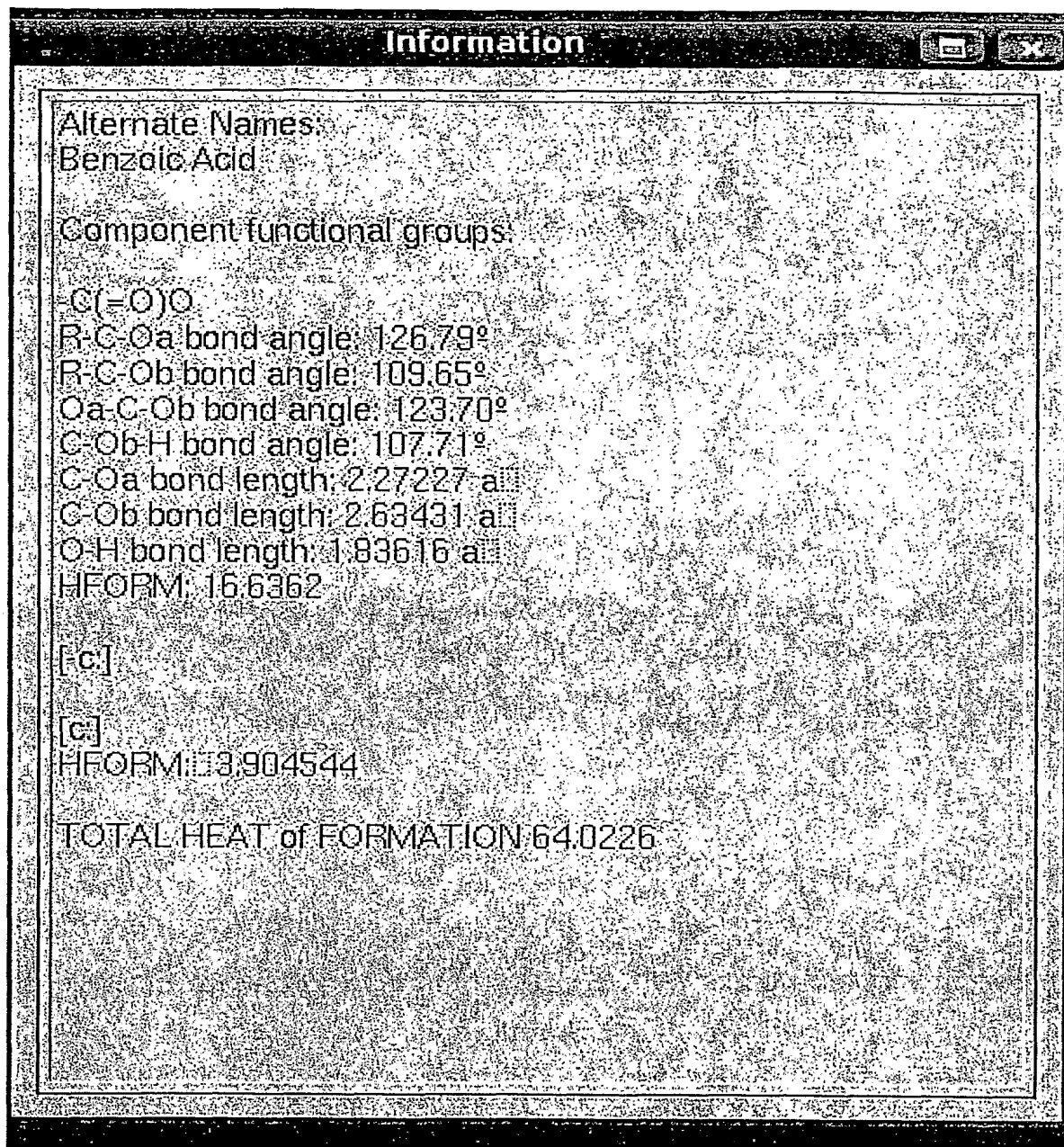


Fig. 3

